

1H-indole-2-carboxylic acid, ethyl ester

Other names:	2-Carbethoxyindole 2-ethoxycarbonylindole Ethyl indole-2-carboxylate Indole-2-carboxylic acid, ethyl ester ethyl 1H-indole-2-carboxylate
Inchi:	InChI=1S/C11H11NO2/c1-2-14-11(13)10-7-8-5-3-4-6-9(8)12-10/h3-7,12H,2H2,1H3
InchiKey:	QQXQAEWRSVZPJM-UHFFFAOYSA-N
Formula:	C11H11NO2
SMILES:	CCOC(=O)c1cc2ccccc2[nH]1
Mol. weight [g/mol]:	189.21

Physical Properties

Property code	Value	Unit	Source
af	0.5885		Cheméo Relay (1.0)
hf	-244.24	kJ/mol	Cheméo Relay (1.0)
hvap	82.26	kJ/mol	Cheméo Relay (1.0)
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-3.60		Cheméo Relay (1.0)
logp	1.863		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3107.63	kPa	Cheméo Relay (1.0, beta)
rinpol	1720.00		NIST Webbook
tb	600.11	K	Cheméo Relay (1.0)
tc	848.40	K	Cheméo Relay (1.0)
tf	402.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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psub	9.88e-04	kPa	348.11	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	8.35e-04	kPa	346.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	6.59e-04	kPa	344.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	5.04e-04	kPa	342.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	4.10e-04	kPa	340.21	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	3.22e-04	kPa	338.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.48e-04	kPa	336.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub	2.03e-04	kPa	334.22	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.57e-04	kPa	332.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.26e-04	kPa	330.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.01e-04	kPa	328.21	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	7.90e-05	kPa	326.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	9.95e-04	kPa	348.11	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	8.08e-04	kPa	346.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub	6.27e-04	kPa	344.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	5.01e-04	kPa	342.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	3.99e-04	kPa	340.21	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	3.12e-04	kPa	338.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.56e-04	kPa	336.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.02e-04	kPa	334.22	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.55e-04	kPa	332.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub	1.23e-04	kPa	330.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	9.80e-05	kPa	328.21	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	7.40e-05	kPa	326.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	9.81e-04	kPa	348.11	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	7.68e-04	kPa	346.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	6.14e-04	kPa	344.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	5.03e-04	kPa	342.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub	3.94e-04	kPa	340.21	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	3.12e-04	kPa	338.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.49e-04	kPa	336.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.96e-04	kPa	334.22	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.54e-04	kPa	332.18	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.22e-04	kPa	330.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	9.10e-05	kPa	328.21	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub

7.40e-05

kPa

326.18

Thermodynamic
properties of alkyl
1H-indole
carboxylate
derivatives: A
combined
experimental and
computational
study

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Thermodynamic properties of alkyl
1H-indole carboxylate derivatives: A
combined experimental and
computational study:
McGowan Method:

<https://www.doi.org/10.1016/j.jct.2016.01.006>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3770501&Units=SI>

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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