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
CAS:	3770-50-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	1.863		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
rinpol	1720.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study:	https://www.doi.org/10.1016/j.jct.2016.01.006
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3770501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
rinpol:	Non-polar retention indices