methyl 1H-indole-3-carboxylate

Other names:	3-methoxycarbonylindole
Inchi:	InChI=1S/C10H9NO2/c1-13-10(12)8-6-11-9-5-3-2-4-7(8)9/h2-6,11H,1H3
InchiKey:	QXAUTQFAWKKNLM-UHFFFAOYSA-N
Formula:	C10H9NO2
SMILES:	COC(=O)c1c[nH]c2ccccc12
Mol. weight [g/mol]:	175.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	1.473		Crippen Method
mcvol	130.260	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	9.60e-04	kPa	375.09	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	8.22e-04	kPa	373.09	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub	7.07e-04	kPa	371.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	5.14e-04	kPa	369.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	4.52e-04	kPa	367.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	3.71e-04	kPa	365.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.84e-04	kPa	363.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.34e-04	kPa	361.11	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.89e-04	kPa	359.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub	1.48e-04	kPa	357.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	1.30e-04	kPa	355.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	1.08e-04	kPa	353.17	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	9.92e-04	kPa	375.09	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	7.99e-04	kPa	373.09	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	6.37e-04	kPa	371.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	5.28e-04	kPa	369.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	

psub	4.39e-04	kPa	367.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	3.51e-04	kPa	365.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.83e-04	kPa	363.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.32e-04	kPa	361.11	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.79e-04	kPa	359.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.54e-04	kPa	357.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.27e-04	kPa	355.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study

psub	9.80e-05	kPa	353.17	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	9.77e-04	kPa	375.09	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	7.92e-04	kPa	373.09	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	6.44e-04	kPa	371.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	5.31e-04	kPa	369.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	4.27e-04	kPa	367.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	
psub	3.47e-04	kPa	365.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study	

psub	2.85e-04	kPa	363.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	2.26e-04	kPa	361.11	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.81e-04	kPa	359.16	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.53e-04	kPa	357.10	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	1.22e-04	kPa	355.12	Thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and computational study
psub	9.70e-05	kPa	353.17	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
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