6-methoxy-dihydroindole

Inchi: InChI=1S/C9H11NO/c1-11-8-3-2-7-4-5-10-9(7)6-8/h2-3,6,10H,4-5H2,1H3
InchiKey: GKFGHNMPMAXWQS-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: COc1ccc2c(c1)NCC2
Mol. weight [g/mol]: 149.19

Physical Properties

Property code	Value	Unit	Source
gf	169.22	kJ/mol	Joback Method
hf	-16.77	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	48.62	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.663		Crippen Method
mcvol	118.900	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2412.00		NIST Webbook
ripol	2384.00		NIST Webbook
tb	524.34	K	Joback Method
tc	756.04	K	Joback Method
tf	392.09	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.73	J/mol×K	524.34	Joback Method
cpg	276.35	J/mol×K	562.96	Joback Method
cpg	289.15	J/mol×K	601.57	Joback Method
cpg	301.15	J/mol×K	640.19	Joback Method

cpg	312.40	J/mol×K	678.81	Joback Method
cpg	322.93	J/mol×K	717.42	Joback Method
cpg	332.78	J/mol×K	756.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R135236&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume