7-ethyl-3-methyl-2-methoxy-2,3-dihydroindole

Inchi: InChI=1S/C12H17NO/c1-4-9-6-5-7-10-8(2)12(14-3)13-11(9)10/h5-8,12-13H,4H2,1-3H3
InchiKey: LNLZPMJJPKIQMN-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCc1cccc2c1NC(OC)C2C
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
gf	179.06	kJ/mol	Joback Method
hf	-119.37	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.750		Crippen Method
mcvol	161.170	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1360.00		NIST Webbook
tb	583.64	K	Joback Method
tc	802.76	K	Joback Method
tf	417.42	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.92	J/mol×K	583.64	Joback Method
cpg	422.98	J/mol×K	620.16	Joback Method
cpg	439.11	J/mol×K	656.68	Joback Method
cpg	454.33	J/mol×K	693.20	Joback Method
cpg	468.67	J/mol×K	729.72	Joback Method
cpg	482.15	J/mol×K	766.24	Joback Method
cpg	494.80	J/mol×K	802.76	Joback Method

Sources

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=R408529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume