6-ethoxy-dihydroindole

Inchi: InChI=1S/C10H13NO/c1-2-12-9-4-3-8-5-6-11-10(8)7-9/h3-4,7,11H,2,5-6H2,1H3
InchiKey: VNQYYRLBJAYXLB-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CCOc1ccc2c(c1)NCC2
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
gf	177.64	kJ/mol	Joback Method
hf	-37.41	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	50.84	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.053		Crippen Method
mcvol	132.990	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2434.00		NIST Webbook
tb	547.22	K	Joback Method
tc	774.61	K	Joback Method
tf	403.36	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.64	J/mol×K	547.22	Joback Method
cpg	322.23	J/mol×K	585.12	Joback Method
cpg	335.95	J/mol×K	623.02	Joback Method
cpg	348.83	J/mol×K	660.91	Joback Method
cpg	360.91	J/mol×K	698.81	Joback Method

cpg	372.24	J/mol×K	736.71	Joback Method
cpg	382.86	J/mol×K	774.61	Joback Method

Sources

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=R135192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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