6-isopropoxy-dihydroindole

Inchi: InChI=1S/C11H15NO/c1-8(2)13-10-4-3-9-5-6-12-11(9)7-10/h3-4,7-8,12H,5-6H2,1-2H3
InchiKey: OMBWDBZPCCLAJF-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CC(C)Oc1ccc2c(c1)NCC2
Mol. weight [g/mol]: 177.24

Physical Properties

Property code	Value	Unit	Source
gf	183.62	kJ/mol	Joback Method
hf	-63.33	kJ/mol	Joback Method
hfus	21.83	kJ/mol	Joback Method
hvap	52.68	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.442		Crippen Method
mcvol	147.080	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1577.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2389.00		NIST Webbook
tb	569.66	K	Joback Method
tc	797.82	K	Joback Method
tf	399.63	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.70	J/mol×K	569.66	Joback Method
cpg	370.53	J/mol×K	607.69	Joback Method
cpg	385.39	J/mol×K	645.71	Joback Method

cpg	399.33	J/mol×K	683.74	Joback Method
cpg	412.39	J/mol×K	721.77	Joback Method
cpg	424.63	J/mol×K	759.79	Joback Method
cpg	436.08	J/mol×K	797.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R135098&Units=SI
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

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