

6-propoxy-dihydroindole

Inchi:	InChI=1S/C11H15NO/c1-2-7-13-10-4-3-9-5-6-12-11(9)8-10/h3-4,8,12H,2,5-7H2,1H3
InchiKey:	DTNUFIMNHTYVOU-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CCCOc1ccc2c(c1)NCC2
Mol. weight [g/mol]:	177.24

Physical Properties

Property code	Value	Unit	Source
gf	186.06	kJ/mol	Joback Method
hf	-58.05	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	53.07	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.443		Crippen Method
mcvol	147.080	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1657.00		NIST Webbook
ripol	2509.00		NIST Webbook
tb	570.10	K	Joback Method
tc	793.29	K	Joback Method
tf	414.63	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.33	J/mol×K	570.10	Joback Method
cpg	369.75	J/mol×K	607.30	Joback Method
cpg	384.26	J/mol×K	644.50	Joback Method
cpg	397.89	J/mol×K	681.70	Joback Method
cpg	410.70	J/mol×K	718.90	Joback Method
cpg	422.72	J/mol×K	756.09	Joback Method
cpg	434.00	J/mol×K	793.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R135241&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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