Noratropine

Inchi: InChI=1S/C16H21NO3/c18-10-15(11-4-2-1-3-5-11)16(19)20-14-8-12-6-7-13(9-14)17-12/h
InchiKey: ATKYNAZQGVYHIB-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: O=C(OC1CC2CCC(C1)N2)C(CO)c1ccccc1
Mol. weight [g/mol]: 275.34
CAS: 16839-98-8

Physical Properties

Property code	Value	Unit	Source
gf	0.37	kJ/mol	Joback Method
hf	-388.60	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	1.589		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	2328.30		NIST Webbook
rinpol	2328.30		NIST Webbook
rinpol	2274.30		NIST Webbook
rinpol	2274.30		NIST Webbook
tb	826.09	K	Joback Method
tc	1050.02	K	Joback Method
tf	544.11	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.73	J/mol×K	826.09	Joback Method
cpg	707.11	J/mol×K	863.41	Joback Method
cpg	721.32	J/mol×K	900.73	Joback Method
cpg	734.41	J/mol×K	938.05	Joback Method
cpg	746.48	J/mol×K	975.38	Joback Method

cpg	757.57	J/mol×K	1012.70	Joback Method
cpg	767.77	J/mol×K	1050.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16839988&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume