Nortilidate

Inchi: InChI=1S/C16H23NO2/c1-3-19-15(18)16(13-9-5-4-6-10-13)12-8-7-11-14(16)17-2/h4-6,9-
InchiKey: WFQQWAVKOIPBTF-UHFFFAOYSA-N
Formula: C16H23NO2
SMILES: CCOC(=O)C1(c2ccccc2)CCCCC1NC
Mol. weight [g/mol]: 261.36

Physical Properties

Property code	Value	Unit	Source
gf	62.97	kJ/mol	Joback Method
hf	-279.15	kJ/mol	Joback Method
hfus	25.73	kJ/mol	Joback Method
hvap	68.05	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.649		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1835.00		NIST Webbook
tb	733.74	K	Joback Method
tc	966.09	K	Joback Method
tf	448.36	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.68	J/mol×K	733.74	Joback Method
cpg	670.42	J/mol×K	772.47	Joback Method
cpg	689.09	J/mol×K	811.19	Joback Method
cpg	706.84	J/mol×K	849.92	Joback Method
cpg	723.82	J/mol×K	888.64	Joback Method
cpg	740.19	J/mol×K	927.37	Joback Method
cpg	756.08	J/mol×K	966.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R489360&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