Ethyl 2-(methylamino)-1-phenyl-3-cyclohexene-1-carbo

Other names:	Nortilidin
	Nortilidine
Inchi:	InChI=1S/C16H21NO2/c1-3-19-15(18)16(13-9-5-4-6-10-13)12-8-7-11-14(16)17-2/h4-7,9-
InchiKey:	PDJZPNKVLDWEKI-UHFFFAOYSA-N
Formula:	C16H21NO2
SMILES:	CCOC(=O)C1(c2ccccc2)CCC=CC1NC
Mol. weight [g/mol]:	259.34
CAS:	38677-94-0

Physical Properties

Property code	Value	Unit	Source
gf	92.93	kJ/mol	Joback Method
hf	-221.37	kJ/mol	Joback Method
hfus	26.95	kJ/mol	Joback Method
hvap	68.34	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.425		Crippen Method
mcvol	214.800	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1859.50		NIST Webbook
rinpol	1859.50		NIST Webbook
tb	732.90	K	Joback Method
tc	967.20	K	Joback Method
tf	449.12	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.46	J/mol×K	732.90	Joback Method
cpg	644.23	J/mol×K	771.95	Joback Method
cpg	661.97	J/mol×K	811.00	Joback Method
cpg	678.85	J/mol×K	850.05	Joback Method
cpg	695.02	J/mol×K	889.10	Joback Method

cpg	710.63	J/mol×K	928.15	Joback Method
cpg	725.85	J/mol×K	967.20	Joback Method

Sources

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=C38677940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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