ETHYL 2-(METHYLAMINO)-1-PHENYL-3-CYCLOHEXENE-

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]: 259.35

Physical Properties

Property code	Value	Unit	Source
hfus	26.95	kJ/mol	Joback Method
log10ws	-2.50		Cheméo Relay (1.0)
logp	2.425		Crippen Method
mcvol	214.800	ml/mol	McGowan Method
rinpol	1859.50		NIST Webbook
rinpol	1859.50		NIST Webbook
tf	377.44	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38677940&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point