Bisnortilidine

Other names:	Bisnortilidin
	Ethyl 2-amino-1-phenyl-3-cyclohexene-1-carboxylate, trans-(+-)-
Inchi:	InChI=1S/C15H19NO2/c1-2-18-14(17)15(11-7-6-10-13(15)16)12-8-4-3-5-9-12/h3-6,8-10,
InchiKey:	BTKAMSWFNMGLGM-UHFFFAOYSA-N
Formula:	C15H19NO2
SMILES:	CCOC(=O)C1(c2ccccc2)CCC=CC1N
Mol. weight [g/mol]:	245.32
CAS:	53948-51-9

Physical Properties

Property code	Value	Unit	Source
gf	61.57	kJ/mol	Joback Method
hf	-220.41	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	70.32	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.165		Crippen Method
mcvol	200.710	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
tb	732.38	K	Joback Method
tc	979.11	K	Joback Method
tf	468.45	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.24	J/mol×K	732.38	Joback Method
cpg	599.38	J/mol×K	773.50	Joback Method
cpg	616.52	J/mol×K	814.62	Joback Method
cpg	632.81	J/mol×K	855.75	Joback Method
cpg	648.45	J/mol×K	896.87	Joback Method

cpg	663.60	J/mol×K	937.99	Joback Method
cpg	678.44	J/mol×K	979.11	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53948519&Units=SI

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