Dicyclomine

Other names:	[1,1'-Bicyclohexyl]-1-carboxylic acid, 2-(diethylamino)ethyl ester
	[Bicyclohexyl]-1-carboxylic acid, 2-(diethylamino)ethyl ester
	Bentyl
	Bentylol
	Dicycloverin
	Dicycloverine
	Diocyl
	Wyovin
Inchi:	InChI=1S/C19H35NO2/c1-3-20(4-2)15-16-22-18(21)19(13-9-6-10-14-19)17-11-7-5-8-12-
InchiKey:	CURUTKGFNZGFSE-UHFFFAOYSA-N
Formula:	C19H35NO2
SMILES:	CCN(CC)CCOC(=O)C1(C2CCCCC2)CCCCC1
Mol. weight [g/mol]:	309.49
CAS:	77-19-0

Physical Properties

Property code	Value	Unit	Source
gf	29.37	kJ/mol	Joback Method
hf	-488.88	kJ/mol	Joback Method
hfus	28.15	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.402		Crippen Method
mcvol	274.270	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2080.00		NIST Webbook

rinpol	2100.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2097.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	762.19	K	Joback Method
tc	976.57	K	Joback Method
tf	447.18	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.49	J/mol×K	762.19	Joback Method
cpg	906.37	J/mol×K	797.92	Joback Method
cpg	929.04	J/mol×K	833.65	Joback Method
cpg	950.63	J/mol×K	869.38	Joback Method
cpg	971.27	J/mol×K	905.11	Joback Method
cpg	991.12	J/mol×K	940.84	Joback Method
cpg	1010.30	J/mol×K	976.57	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77190&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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