Azacyclonol

Other names: 4-(Diphenylhydroxymethyl)piperidine
4-Piperidinemethanol, «alpha»,«alpha»-diphenyl-
4-Piperidinemethanol, Â«alphaÂ»,Â«alphaÂ»-diphenyl-
Ataractan
Azacyclonal
Azacyklonol
Calmeran
Diphenyl-4-piperidylmethanol
Frenoton
Frenquel
MER 17
Psychosan
di(phenyl)-piperidin-4-ylmethanol
«alpha»,«alpha»-Diphenyl-4-piperidinemethanol
«alpha»-(4-Piperidyl)benzhydrol
«gamma»-Pipradol
Â«alphaÂ»,Â«alphaÂ»-Diphenyl-4-piperidinemethanol
Â«alphaÂ»-(4-Piperidyl)benzhydrol
Â«gammaÂ»-Pipradol

Inchi: InChI=1S/C18H21NO/c20-18(15-7-3-1-4-8-15,16-9-5-2-6-10-16)17-11-13-19-14-12-17/h1

InchiKey: ZMISODWVFHHWNR-UHFFFAOYSA-N

Formula: C18H21NO

SMILES: OC(c1ccccc1)(c1ccccc1)C1CCNCC1

Mol. weight [g/mol]: 267.37

CAS: 115-46-8

Physical Properties

Property code	Value	Unit	Source
gf	303.68	kJ/mol	Joback Method
hf	-10.64	kJ/mol	Joback Method
hfus	28.56	kJ/mol	Joback Method
hvap	82.78	kJ/mol	Joback Method
log10ws	-1.39		Aqueous Solubility Prediction Method
logp	2.922		Crippen Method
mcvol	221.950	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method

rinpol	2220.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	821.65	K	Joback Method
tc	1072.96	K	Joback Method
tf	433.32	K	Aqueous Solubility Prediction Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.83	J/mol×K	821.65	Joback Method
cpg	702.58	J/mol×K	863.54	Joback Method
cpg	717.81	J/mol×K	905.42	Joback Method
cpg	731.66	J/mol×K	947.31	Joback Method
cpg	744.28	J/mol×K	989.19	Joback Method
cpg	755.80	J/mol×K	1031.08	Joback Method
cpg	766.35	J/mol×K	1072.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115468&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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