

Pipradrol

Other names:	2-Piperidinemethanol, «alpha»,«alpha»-diphenyl- 2-Piperidinemethanol, Â«alphaÂ»,Â«alphaÂ»-diphenyl- A-(2-piperidyl)-benzohydrol Detaril Gerodyl MRD 108 Pipradol Pipralon Piridrol Pyridrol Pyridrole alpha-(2-Piperidyl)-benzohydrol alpha-Pipradol di(phenyl)-piperidin-2-ylmethanol «alpha»,«alpha»-Diphenyl-2-piperidinemethanol «alpha»,«alpha»-Diphenyl-«alpha»-(2-piperidyl)methanol «alpha»-(2-Piperidyl)benzhydrol «alpha»-Pipradol Â«alphaÂ»,Â«alphaÂ»-Diphenyl-2-piperidinemethanol Â«alphaÂ»,Â«alphaÂ»-Diphenyl-Â«alphaÂ»-(2-piperidyl)methanol Â«alphaÂ»-(2-Piperidyl)benzhydrol Â«alphaÂ»-Pipradol
Inchi:	InChI=1S/C18H21NO/c20-18(15-9-3-1-4-10-15,16-11-5-2-6-12-16)17-13-7-8-14-19-17/h
InchiKey:	XSWHNYGMWWVAIE-UHFFFAOYSA-N
Formula:	C18H21NO
SMILES:	OC(c1ccccc1)(c1ccccc1)C1CCCCN1
Mol. weight [g/mol]:	267.37
CAS:	467-60-7

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	-1.90		Aqueous Solubility Prediction Method

logp	3.065		Crippen Method
mcvol	221.950	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	821.65	K	Joback Method
tc	1072.96	K	Joback Method
tf	521.11	K	Joback 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=C467607&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/AqueousDataset002.xlsx
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

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