PERHEXILINE

Other names: Perhexiline
2-(2,2-Dicyclohexylethyl)piperidine
Perhexilene
Inchi: InChI=1S/C19H35N/c1-3-9-16(10-4-1)19(17-11-5-2-6-12-17)15-18-13-7-8-14-20-18/h16-
InchiKey: CYXKNKQEMFBLER-UHFFFAOYSA-N
Formula: C19H35N
SMILES: C1CCC(C(CC2CCCCN2)C2CCCCC2)CC1
Mol. weight [g/mol]: 277.50

Physical Properties

Property code	Value	Unit	Source
hfus	26.54	kJ/mol	Joback Method
hvap	92.69	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.39		Cheméo Relay (1.0)
logp	5.295		Crippen Method
mcvol	255.970	ml/mol	McGowan Method
rinpol	2138.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	651.23	K	Cheméo Relay (1.0)
tf	351.21	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.34	J/mol×K	740.88	Joback Method
cpg	868.62	J/mol×K	781.94	Joback Method
cpg	895.53	J/mol×K	823.00	Joback Method
cpg	920.16	J/mol×K	864.06	Joback Method
cpg	942.60	J/mol×K	905.13	Joback Method
cpg	962.93	J/mol×K	946.19	Joback Method
cpg	981.25	J/mol×K	987.25	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C6621472&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point