Pencycuron

Other names:	1-[(4-chlorophenyl)methyl]-1-cyclopentyl-3-phenylurea
	Bay NTN 19701
	Monceren
	N-((4-Chlorophenyl)methyl)-N-cyclopentyl-N'-phenylurea
	Trotis
	Urea, N-[(4-chlorophenyl)methyl]-N-cyclopentyl-N'-phenyl-
	[(Chlorophenyl)-methyl]-N-cyclopentyl-N'-phenylurea
Inchi:	InChI=1S/C19H21ClN2O/c20-16-12-10-15(11-13-16)14-22(18-8-4-5-9-18)19(23)21-17-6-
InchiKey:	OGYFATSSENRIKG-UHFFFAOYSA-N
Formula:	C19H21ClN2O
SMILES:	O=C(Nc1ccccc1)N(Cc1ccc(Cl)cc1)C1CCCC1
Mol. weight [g/mol]:	328.84
CAS:	66063-05-6

Physical Properties

Property code	Value	Unit	Source
gf	420.16	kJ/mol	Joback Method
hf	79.26	kJ/mol	Joback Method
hfus	40.51	kJ/mol	Joback Method
hvap	82.97	kJ/mol	Joback Method
log10ws	-5.92		Estimated Solubility Method
log10ws	-5.91		Aqueous Solubility Prediction Method
logp	5.317		Crippen Method
mcvol	253.960	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	861.65	K	Joback Method
tc	1109.11	K	Joback Method
tf	545.13	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.17	J/mol×K	861.65	Joback Method
cpg	782.97	J/mol×K	902.89	Joback Method
cpg	797.39	J/mol×K	944.14	Joback Method
cpg	810.57	J/mol×K	985.38	Joback Method
cpg	822.64	J/mol×K	1026.62	Joback Method
cpg	833.75	J/mol×K	1067.86	Joback Method
cpg	844.03	J/mol×K	1109.11	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66063056&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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