N,N'-DI(P-CHLOROBENZYL)UREA

Other names: Urea, N,N'-bis[(4-chlorophenyl)methyl]-
Urea, 1,3-bis(p-chlorobenzyl)-
Inchi: InChI=1S/C15H14Cl2N2O/c16-13-5-1-11(2-6-13)9-18-15(20)19-10-12-3-7-14(17)8-4-12/h
InchiKey: UQCDPZIXWSDDRU-UHFFFAOYSA-N
Formula: C15H14Cl2N2O
SMILES: O=C(NCc1ccc(Cl)cc1)NCc1ccc(Cl)cc1
Mol. weight [g/mol]: 309.20

Physical Properties

Property code	Value	Unit	Source
hfus	42.10	kJ/mol	Joback Method
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-4.73		Cheméo Relay (1.0)
logp	3.993		Crippen Method
mcvol	220.700	ml/mol	McGowan Method
tb	646.40	K	Cheméo Relay (1.0)
tf	399.86	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.91	J/mol×K	834.99	Joback Method
cpg	599.57	J/mol×K	875.34	Joback Method
cpg	610.20	J/mol×K	915.69	Joback Method
cpg	619.87	J/mol×K	956.04	Joback Method
cpg	628.66	J/mol×K	996.39	Joback Method
cpg	636.64	J/mol×K	1036.74	Joback Method
cpg	643.90	J/mol×K	1077.09	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92550157&Units=SI
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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point