Urea, 1,1'-o-phenylenebis[3-(2-chloroethyl)-

Inchi: InChI=1S/C12H16Cl2N4O2/c13-5-7-15-11(19)17-9-3-1-2-4-10(9)18-12(20)16-8-6-14/h1-
InchiKey: JAOPEDLQYKNPMS-UHFFFAOYSA-N
Formula: C12H16Cl2N4O2
SMILES: O=C(NCCCl)Nc1ccccc1NC(=O)NCCCl
Mol. weight [g/mol]: 319.19
CAS: 13908-65-1

Physical Properties

Property code	Value	Unit	Source
gf	228.80	kJ/mol	Joback Method
hf	-108.71	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.407		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	888.90	K	Joback Method
tc	1111.44	K	Joback Method
tf	634.28	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.30	J/mol×K	888.90	Joback Method
cpg	642.04	J/mol×K	925.99	Joback Method
cpg	650.93	J/mol×K	963.08	Joback Method
cpg	659.03	J/mol×K	1000.17	Joback Method
cpg	666.39	J/mol×K	1037.26	Joback Method
cpg	673.06	J/mol×K	1074.35	Joback Method
cpg	679.10	J/mol×K	1111.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908651&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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