Urea, 1-(2-chloroethyl)-3-(alpha,alpha-dimethylpheneth

Inchi: InChI=1S/C13H19ClN2O/c1-13(2,16-12(17)15-9-8-14)10-11-6-4-3-5-7-11/h3-7H,8-10H2,

InchiKey: KNNXGYCEUVHRSD-UHFFFAOYSA-N

Formula: C13H19ClN2O

SMILES: CC(C)(Cc1ccccc1)NC(=O)NCCCl

Mol. weight [g/mol]: 254.76

CAS: 33082-80-3

Physical Properties

Property code	Value	Unit	Source
gf	211.76	kJ/mol	Joback Method
hf	-105.25	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.546		Crippen Method
mcvol	204.040	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
tb	711.93	K	Joback Method
tc	930.90	K	Joback Method
tf	450.28	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.38	J/mol×K	711.93	Joback Method
cpg	568.87	J/mol×K	748.42	Joback Method
cpg	582.30	J/mol×K	784.92	Joback Method
cpg	594.74	J/mol×K	821.41	Joback Method
cpg	606.29	J/mol×K	857.91	Joback Method
cpg	617.00	J/mol×K	894.40	Joback Method
cpg	626.96	J/mol×K	930.90	Joback Method

Sources

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=C33082803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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