Urea, 1-(2-chlorocyclohexyl)-3-methyl-, trans-

Inchi: InChI=1S/C8H15ClN2O/c1-10-8(12)11-7-5-3-2-4-6(7)9/h6-7H,2-5H2,1H3,(H2,10,11,12)/t

InchiKey: WYNIPLSOPDHHQX-BQBZGAKWSA-N

Formula: C8H15ClN2O

SMILES: CNC(=O)NC1CCCCC1Cl

Mol. weight [g/mol]: 190.67

CAS: 13908-81-1

Physical Properties

Property code	Value	Unit	Source
gf	71.15	kJ/mol	Joback Method
hf	-195.85	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	57.53	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.465		Crippen Method
mcvol	146.490	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	588.96	K	Joback Method
tc	808.02	K	Joback Method
tf	368.23	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.97	J/mol×K	588.96	Joback Method
cpg	384.86	J/mol×K	625.47	Joback Method
cpg	399.76	J/mol×K	661.98	Joback Method
cpg	413.69	J/mol×K	698.49	Joback Method
cpg	426.67	J/mol×K	735.00	Joback Method
cpg	438.73	J/mol×K	771.51	Joback Method
cpg	449.89	J/mol×K	808.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908811&Units=SI
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

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