Urea, 1-(2-chloroethyl)-3-cycloheptyl-

Inchi: InChI=1S/C10H19ClN2O/c11-7-8-12-10(14)13-9-5-3-1-2-4-6-9/h9H,1-8H2,(H2,12,13,14)
InchiKey: BKCHWJUBSGHNQU-UHFFFAOYSA-N
Formula: C10H19ClN2O
SMILES: O=C(NCCCl)NC1CCCCCC1
Mol. weight [g/mol]: 218.72
CAS: 13908-27-5

Physical Properties

Property code	Value	Unit	Source
gf	83.60	kJ/mol	Joback Method
hf	-222.95	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.247		Crippen Method
mcvol	174.670	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	643.66	K	Joback Method
tc	862.14	K	Joback Method
tf	391.49	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.78	J/mol×K	643.66	Joback Method
cpg	487.07	J/mol×K	680.07	Joback Method
cpg	503.21	J/mol×K	716.49	Joback Method
cpg	518.23	J/mol×K	752.90	Joback Method
cpg	532.18	J/mol×K	789.32	Joback Method
cpg	545.06	J/mol×K	825.73	Joback Method
cpg	556.93	J/mol×K	862.14	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=C13908275&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