

Urea, 1-acetyl-1,3-dicyclohexyl-

Inchi:	InChI=1S/C15H26N2O2/c1-12(18)17(14-10-6-3-7-11-14)15(19)16-13-8-4-2-5-9-13/h13-1
InchiKey:	KSYCMDUQWWSFNO-UHFFFAOYSA-N
Formula:	C15H26N2O2
SMILES:	CC(=O)N(C(=O)NC1CCCCC1)C1CCCCC1
Mol. weight [g/mol]:	266.38
CAS:	42965-13-9

Physical Properties

Property code	Value	Unit	Source
gf	66.65	kJ/mol	Joback Method
hf	-348.45	kJ/mol	Joback Method
hfus	29.59	kJ/mol	Joback Method
hvap	71.81	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.210		Crippen Method
mcvol	223.590	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
tb	752.05	K	Joback Method
tc	979.61	K	Joback Method
tf	458.56	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.74	J/molxK	752.05	Joback Method
cpg	730.25	J/molxK	789.98	Joback Method
cpg	749.13	J/molxK	827.90	Joback Method
cpg	766.45	J/molxK	865.83	Joback Method
cpg	782.29	J/molxK	903.76	Joback Method
cpg	796.72	J/molxK	941.69	Joback Method
cpg	809.80	J/molxK	979.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C42965139&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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