2-Butenamide, N,N-dicyclohexyl-

Other names: N,N-Dicyclohexyl crotonamide
Inchi: InChI=1S/C16H27NO/c1-2-9-16(18)17(14-10-5-3-6-11-14)15-12-7-4-8-13-15/h2,9,14-15H
InchiKey: YPAZZFZYOAKJJY-XNWCZRBMSA-N
Formula: C16H27NO
SMILES: CC=CC(=O)N(C1CCCCC1)C1CCCCC1
Mol. weight [g/mol]: 249.39
CAS: 55955-94-7

Physical Properties

Property code	Value	Unit	Source
gf	194.82	kJ/mol	Joback Method
hf	-192.76	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	60.81	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.057		Crippen Method
mcvol	221.830	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
tb	675.05	K	Joback Method
tc	903.10	K	Joback Method
tf	362.16	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.11	J/mol×K	675.05	Joback Method
cpg	679.19	J/mol×K	713.06	Joback Method
cpg	701.53	J/mol×K	751.07	Joback Method
cpg	722.23	J/mol×K	789.08	Joback Method
cpg	741.39	J/mol×K	827.08	Joback Method
cpg	759.07	J/mol×K	865.09	Joback Method
cpg	775.39	J/mol×K	903.10	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=C55955947&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