Propanamide, N-cyclohexyl-2,2-dimethyl

Inchi: InChI=1S/C11H21NO/c1-11(2,3)10(13)12-9-7-5-4-6-8-9/h9H,4-8H2,1-3H3,(H,12,13)
InchiKey: IDQKJTPEUNXEDP-UHFFFAOYSA-N
Formula: C11H21NO
SMILES: CC(C)(C)C(=O)NC1CCCCC1
Mol. weight [g/mol]: 183.29

Physical Properties

Property code	Value	Unit	Source
gf	29.50	kJ/mol	Joback Method
hf	-283.91	kJ/mol	Joback Method
hfus	15.36	kJ/mol	Joback Method
hvap	52.39	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.481		Crippen Method
mcvol	166.540	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1308.00		NIST Webbook
tb	571.44	K	Joback Method
tc	788.72	K	Joback Method
tf	326.12	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.39	J/mol×K	571.44	Joback Method
cpg	455.15	J/mol×K	607.65	Joback Method
cpg	473.62	J/mol×K	643.87	Joback Method
cpg	490.88	J/mol×K	680.08	Joback Method
cpg	506.97	J/mol×K	716.30	Joback Method
cpg	521.95	J/mol×K	752.51	Joback Method
cpg	535.88	J/mol×K	788.72	Joback Method

Sources

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=R50878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume