

Butanamide, N-cyclohexyl-3-methyl

Inchi:	InChI=1S/C11H21NO/c1-9(2)8-11(13)12-10-6-4-3-5-7-10/h9-10H,3-8H2,1-2H3,(H,12,13)
InchiKey:	KDOWYZAXEZQVBH-UHFFFAOYSA-N
Formula:	C11H21NO
SMILES:	CC(C)CC(=O)NC1CCCCC1
Mol. weight [g/mol]:	183.29

Physical Properties

Property code	Value	Unit	Source
gf	24.22	kJ/mol	Joback Method
hf	-280.44	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	53.30	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.481		Crippen Method
mcvol	166.540	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinqol	1496.00		NIST Webbook
tb	574.23	K	Joback Method
tc	783.28	K	Joback Method
tf	308.70	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.78	J/molxK	574.23	Joback Method
cpg	451.83	J/molxK	609.07	Joback Method
cpg	469.80	J/molxK	643.91	Joback Method
cpg	486.70	J/molxK	678.75	Joback Method
cpg	502.57	J/molxK	713.60	Joback Method
cpg	517.45	J/molxK	748.44	Joback Method
cpg	531.36	J/molxK	783.28	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=R50476&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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