

Butanamide, N-cyclohexyl-

Other names:	Butyramide, N-cyclohexyl- N-Cyclohexylbutyramide
Inchi:	InChI=1S/C10H19NO/c1-2-6-10(12)11-9-7-4-3-5-8-9/h9H,2-8H2,1H3,(H,11,12)
InchiKey:	MIUPVUSAABKKQX-UHFFFAOYSA-N
Formula:	C10H19NO
SMILES:	CCCC(=O)NC1CCCCC1
Mol. weight [g/mol]:	169.26
CAS:	1199-87-7

Physical Properties

Property code	Value	Unit	Source
gf	18.24	kJ/mol	Joback Method
hf	-254.52	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	51.47	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.235		Crippen Method
mcvol	152.450	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1459.00		NIST Webbook
tb	551.79	K	Joback Method
tc	759.76	K	Joback Method
tf	312.43	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.44	J/mol×K	551.79	Joback Method
cpg	400.51	J/mol×K	586.45	Joback Method
cpg	417.56	J/mol×K	621.11	Joback Method
cpg	433.63	J/mol×K	655.78	Joback Method
cpg	448.75	J/mol×K	690.44	Joback Method
cpg	462.94	J/mol×K	725.10	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=C1199877&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

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