

# 2-Carboxamide, 4-cyclohexyl butyric acid

<b>Inchi:</b>	InChI=1S/C11H19NO3/c12-10(13)9(11(14)15)7-6-8-4-2-1-3-5-8/h8-9H,1-7H2,(H2,12,13)
<b>InchiKey:</b>	SKOGCXVYDHZWNC-UHFFFAOYSA-N
<b>Formula:</b>	C11H19NO3
<b>SMILES:</b>	NC(=O)C(CCC1CCCCC1)C(=O)O
<b>Mol. weight [g/mol]:</b>	213.27
<b>CAS:</b>	116346-21-5

## Physical Properties

Property code	Value	Unit	Source
gf	-264.46	kJ/mol	Joback Method
hf	-564.93	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.533		Crippen Method
mcvol	173.980	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	742.64	K	Joback Method
tc	952.03	K	Joback Method
tf	450.05	K	Joback Method
vc	0.638	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.13	J/molxK	742.64	Joback Method
cpg	539.66	J/molxK	777.54	Joback Method
cpg	552.25	J/molxK	812.44	Joback Method
cpg	563.93	J/molxK	847.34	Joback Method
cpg	574.73	J/molxK	882.24	Joback Method
cpg	584.68	J/molxK	917.13	Joback Method
cpg	593.82	J/molxK	952.03	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346215&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346215&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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