

Propanamide, N-(1-oxopropyl)-

Other names:	Dipropionamide
Inchi:	InChI=1S/C6H11NO2/c1-3-5(8)7-6(9)4-2/h3-4H2,1-2H3,(H,7,8,9)
InchiKey:	GOJDSMIXPMMHPO-UHFFFAOYSA-N
Formula:	C6H11NO2
SMILES:	CCC(=O)NC(=O)CC
Mol. weight [g/mol]:	129.16
CAS:	6050-26-6

Physical Properties

Property code	Value	Unit	Source
chs	-3382.24	kJ/mol	NIST Webbook
gf	-168.81	kJ/mol	Joback Method
hf	-338.86	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	48.88	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.449		Crippen Method
mcvol	108.520	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	488.20	K	NIST Webbook
tc	686.85	K	Joback Method
tf	309.90	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.35	J/molxK	494.59	Joback Method
cpg	244.44	J/molxK	526.63	Joback Method
cpg	254.05	J/molxK	558.68	Joback Method
cpg	263.20	J/molxK	590.72	Joback Method
cpg	271.90	J/molxK	622.76	Joback Method
cpg	280.15	J/molxK	654.81	Joback Method
cpg	287.97	J/molxK	686.85	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=C6050266&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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

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