

L-Alanine, N-acetyl-, methyl ester

Inchi:	InChI=1S/C6H11NO3/c1-4(6(9)10-3)7-5(2)8/h4H,1-3H3,(H,7,8)/t4-/m1/s1
InchiKey:	FQGVVDYNRHNTCK-SCSAIBSYSA-N
Formula:	C6H11NO3
SMILES:	COC(=O)C(C)NC(C)=O
Mol. weight [g/mol]:	145.16
CAS:	3619-02-1

Physical Properties

Property code	Value	Unit	Source
gf	-276.25	kJ/mol	Joback Method
hf	-476.36	kJ/mol	Joback Method
hfus	17.26	kJ/mol	Joback Method
hvap	50.90	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.316		Crippen Method
mcvol	114.390	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	516.57	K	Joback Method
tc	711.62	K	Joback Method
tf	317.13	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.69	J/molxK	516.57	Joback Method
cpg	266.93	J/molxK	549.08	Joback Method
cpg	276.73	J/molxK	581.59	Joback Method
cpg	286.08	J/molxK	614.10	Joback Method
cpg	294.98	J/molxK	646.61	Joback Method
cpg	303.44	J/molxK	679.11	Joback Method
cpg	311.45	J/molxK	711.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C3619021&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
mccvol:	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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