

L-Alanine, ethyl ester

Other names:	Alanine, ethyl ester, L- Alanine ethyl ester L-«alpha»-Alanine ethyl ester ethyl alaninate ethyl L-alaninate
Inchi:	InChI=1S/C5H11NO2/c1-3-8-5(7)4(2)6/h4H,3,6H2,1-2H3/t4-/m1/s1
InchiKey:	ROBXZHNBBCHEIQ-SCSAIBSYSA-N
Formula:	C5H11NO2
SMILES:	CCOC(=O)C(C)N
Mol. weight [g/mol]:	117.15
CAS:	3082-75-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.69	kJ/mol	Joback Method
hf	-362.82	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	-0.103		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	462.18	K	Joback Method
tc	659.06	K	Joback Method
tf	286.53	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.74	J/molxK	462.18	Joback Method
cpg	220.39	J/molxK	494.99	Joback Method
cpg	229.66	J/molxK	527.81	Joback Method
cpg	238.56	J/molxK	560.62	Joback Method

cpg	247.09	J/mol×K	593.43	Joback Method
cpg	255.24	J/mol×K	626.24	Joback Method
cpg	263.02	J/mol×K	659.06	Joback Method

Sources

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=C3082755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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