DL-Alanine, N-DL-alanyl-

Other names:	Alanine, N-DL-alanyl-, DL- DL-Ala-DL-Ala DL-Alanyl-DL-alanine N-DL-Alanyl-DL-alanine
Inchi:	InChI=1S/C6H12N2O3/c1-3(7)5(9)8-4(2)6(10)11/h3-4H,7H2,1-2H3,(H,8,9)(H,10,11)
InchiKey:	DEFJQIDDEAULHB-UHFFFAOYSA-N
Formula:	C6H12N2O3
SMILES:	CC(N)C(=O)NC(C)C(=O)O
Mol. weight [g/mol]:	160.17
CAS:	2867-20-1

Physical Properties

Property code	Value	Unit	Source
chs	-3267.50 ± 1.80	kJ/mol	NIST Webbook
gf	-244.06	kJ/mol	Joback Method
hf	-467.86	kJ/mol	Joback Method
hfs	-807.30 ± 1.90	kJ/mol	NIST Webbook
hfus	21.83	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	-1.077		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	658.42	K	Joback Method
tc	855.69	K	Joback Method
tf	423.98	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.27	J/mol×K	658.42	Joback Method
cpg	340.11	J/mol×K	691.30	Joback Method
cpg	348.42	J/mol×K	724.18	Joback Method

cpg	356.22	J/mol×K	757.06	Joback Method
cpg	363.53	J/mol×K	789.94	Joback Method
cpg	370.36	J/mol×K	822.82	Joback Method
cpg	376.72	J/mol×K	855.69	Joback Method
cps	189.00	J/mol×K	298.00	NIST Webbook
hfust	33.20	kJ/mol	483.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2867201&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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