DL-Valine, N-acetyl-, methyl ester

Other names: N-Acetyl-DL-valine methyl ester
Inchi: InChI=1S/C8H15NO3/c1-5(2)7(8(11)12-4)9-6(3)10/h5,7H,1-4H3,(H,9,10)
InchiKey: KCHNPFJMSOGXIT-UHFFFAOYSA-N
Formula: C8H15NO3
SMILES: COC(=O)C(NC(C)=O)C(C)C
Mol. weight [g/mol]: 173.21
CAS: 52152-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-261.85	kJ/mol	Joback Method
hf	-522.92	kJ/mol	Joback Method
hfus	18.92	kJ/mol	Joback Method
hvap	54.96	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.320		Crippen Method
mcvol	142.570	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1249.40		NIST Webbook
ripol	1960.00		NIST Webbook
tb	561.89	K	Joback Method
tc	755.87	K	Joback Method
tf	324.67	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.20	J/mol×K	561.89	Joback Method
cpg	358.67	J/mol×K	594.22	Joback Method
cpg	370.56	J/mol×K	626.55	Joback Method
cpg	381.86	J/mol×K	658.88	Joback Method
cpg	392.57	J/mol×K	691.21	Joback Method
cpg	402.72	J/mol×K	723.54	Joback Method

cpg	412.29	J/mol×K	755.87	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=C52152473&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume