L-Valine, ethyl ester

Other names:	Valine, ethyl ester, L-
	Valine ethyl ester
	Ethyl L-valinate
	Ethyl valinate
	Ethyl butanoate, 2-amino-3-methyl
Inchi:	InChI=1S/C7H15NO2/c1-4-10-7(9)6(8)5(2)3/h5-6H,4,8H2,1-3H3
InchiKey:	BQIVJVAZDJHDJF-UHFFFAOYSA-N
Formula:	C7H15NO2
SMILES:	CCOC(=O)C(N)C(C)C
Mol. weight [g/mol]:	145.20
CAS:	17431-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-164.29	kJ/mol	Joback Method
hf	-409.38	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.533		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	1017.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	992.00		NIST Webbook
tb	507.50	K	Joback Method
tc	703.81	K	Joback Method
tf	294.07	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	294.09	J/mol×K	507.50	Joback Method
cpg	306.40	J/mol×K	540.22	Joback Method
cpg	318.17	J/mol×K	572.94	Joback Method
cpg	329.42	J/mol×K	605.65	Joback Method
cpg	340.15	J/mol×K	638.37	Joback Method
cpg	350.36	J/mol×K	671.09	Joback Method
cpg	360.05	J/mol×K	703.81	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=C17431037&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume