L-Valine, methyl ester

Other names:	Valine, methyl ester, L- (+)-L-Valine methyl ester Methyl valine Methyl L-valinate Valine methyl ester Val, methyl ester
Inchi:	InChI=1S/C6H13NO2/c1-4(2)5(7)6(8)9-3/h4-5H,7H2,1-3H3/t5-/m1/s1
InchiKey:	CEMZBWPSKYISTN-RXMQYKEDSA-N
Formula:	C6H13NO2
SMILES:	COC(=O)C(N)C(C)C
Mol. weight [g/mol]:	131.17
CAS:	4070-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-172.71	kJ/mol	Joback Method
hf	-388.74	kJ/mol	Joback Method
hfus	12.23	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.143		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
rinpol	1017.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1024.00		NIST Webbook
tb	484.62	K	Joback Method
tc	683.50	K	Joback Method
tf	282.80	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	251.46	J/mol×K	484.62	Joback Method
cpg	262.67	J/mol×K	517.77	Joback Method
cpg	273.40	J/mol×K	550.91	Joback Method
cpg	283.67	J/mol×K	584.06	Joback Method
cpg	293.47	J/mol×K	617.21	Joback Method
cpg	302.81	J/mol×K	650.35	Joback Method
cpg	311.68	J/mol×K	683.50	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=C4070488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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