

Valeric acid, 3-hydroxy-2,2,4-trimethyl-

Inchi:	InChI=1S/C8H16O3/c1-5(2)6(9)8(3,4)7(10)11/h5-6,9H,1-4H3,(H,10,11)
InchiKey:	OJLBQZJKORZRDZ-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CC(C)C(O)C(C)(C)C(=O)O
Mol. weight [g/mol]:	160.21
CAS:	35763-45-2

Physical Properties

Property code	Value	Unit	Source
gf	-388.12	kJ/mol	Joback Method
hf	-644.80	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.114		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	616.56	K	Joback Method
tc	793.88	K	Joback Method
tf	323.91	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.84	J/mol×K	616.56	Joback Method
cpg	374.94	J/mol×K	646.11	Joback Method
cpg	384.50	J/mol×K	675.67	Joback Method
cpg	393.54	J/mol×K	705.22	Joback Method
cpg	402.08	J/mol×K	734.77	Joback Method
cpg	410.16	J/mol×K	764.32	Joback Method
cpg	417.80	J/mol×K	793.88	Joback Method
dvisc	0.0429980	Pa×s	323.91	Joback Method
dvisc	0.0055542	Pa×s	372.69	Joback Method

dvisc	0.0011522	Pa×s	421.46	Joback Method
dvisc	0.0003312	Pa×s	470.24	Joback Method
dvisc	0.0001204	Pa×s	519.01	Joback Method
dvisc	0.0000520	Pa×s	567.78	Joback Method
dvisc	0.0000257	Pa×s	616.56	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=C35763452&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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