

Valeric acid, 4-hydroxy-2,2,4-trimethyl, gamma-lactone

Inchi:	InChI=1S/C8H14O2/c1-7(2)5-8(3,4)10-6(7)9/h5H2,1-4H3
InchiKey:	DTPSINDCVZJYPO-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC1(C)CC(C)(C)C(=O)O1
Mol. weight [g/mol]:	142.20
CAS:	4237-83-6

Physical Properties

Property code	Value	Unit	Source
gf	-174.37	kJ/mol	Joback Method
hf	-407.53	kJ/mol	Joback Method
hfus	6.37	kJ/mol	Joback Method
hvap	39.81	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.738		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	488.30	K	Joback Method
tc	717.80	K	Joback Method
tf	329.17	K	Joback Method
vc	0.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.20	J/mol×K	488.30	Joback Method
cpg	294.96	J/mol×K	526.55	Joback Method
cpg	309.57	J/mol×K	564.80	Joback Method
cpg	323.23	J/mol×K	603.05	Joback Method
cpg	336.12	J/mol×K	641.30	Joback Method
cpg	348.45	J/mol×K	679.55	Joback Method
cpg	360.40	J/mol×K	717.80	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=C4237836&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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