

Valeric acid, 2,2,4-trimethyl-3-oxo-, butyl ester

Inchi:	InChI=1S/C12H22O3/c1-6-7-8-15-11(14)12(4,5)10(13)9(2)3/h9H,6-8H2,1-5H3
InchiKey:	IOCDAKOKYMMTRL-UHFFFAOYSA-N
Formula:	C12H22O3
SMILES:	CCCCOC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]:	214.30
CAS:	4447-69-2

Physical Properties

Property code	Value	Unit	Source
gf	-312.28	kJ/mol	Joback Method
hf	-662.42	kJ/mol	Joback Method
hfus	20.29	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.581		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
tb	600.45	K	Joback Method
tc	790.59	K	Joback Method
tf	334.51	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.20	J/molxK	600.45	Joback Method
cpg	507.94	J/molxK	632.14	Joback Method
cpg	522.86	J/molxK	663.83	Joback Method
cpg	536.98	J/molxK	695.52	Joback Method
cpg	550.33	J/molxK	727.21	Joback Method
cpg	562.93	J/molxK	758.90	Joback Method
cpg	574.81	J/molxK	790.59	Joback Method
dvisc	0.0035399	Paxs	334.51	Joback Method
dvisc	0.0015652	Paxs	378.83	Joback Method

dvisc	0.0008211	Paxs	423.16	Joback Method
dvisc	0.0004868	Paxs	467.48	Joback Method
dvisc	0.0003160	Paxs	511.80	Joback Method
dvisc	0.0002197	Paxs	556.13	Joback Method
dvisc	0.0001612	Paxs	600.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4447692&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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