

Ethylene glycol mono-2,2,4-trimethyl-3-oxovalerate

Inchi:	InChI=1S/C10H18O4/c1-7(2)8(12)10(3,4)9(13)14-6-5-11/h7,11H,5-6H2,1-4H3
InchiKey:	NARNUWZBBOTQQX-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CC(C)C(=O)C(C)(C)C(=O)OCCO
Mol. weight [g/mol]:	202.25
CAS:	116659-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-465.94	kJ/mol	Joback Method
hf	-773.37	kJ/mol	Joback Method
hfus	19.19	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	0.773		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	646.87	K	Joback Method
tc	832.00	K	Joback Method
tf	372.79	K	Joback Method
vc	0.627	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.17	J/molxK	646.87	Joback Method
cpg	503.85	J/molxK	801.15	Joback Method
cpg	494.33	J/molxK	770.29	Joback Method
cpg	484.22	J/molxK	739.44	Joback Method
cpg	473.51	J/molxK	708.58	Joback Method
cpg	462.17	J/molxK	677.73	Joback Method
cpg	512.79	J/molxK	832.00	Joback Method
dvisc	0.0000532	Paxs	646.87	Joback Method
dvisc	0.0000838	Paxs	601.19	Joback Method

dvisc	0.0001421	Paxs	555.51	Joback Method
dvisc	0.0002650	Paxs	509.83	Joback Method
dvisc	0.0005589	Paxs	464.15	Joback Method
dvisc	0.0013868	Paxs	418.47	Joback Method
dvisc	0.0042998	Paxs	372.79	Joback Method

Sources

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=C116659531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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