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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.17	J/mol×K	646.87	Joback Method
cpg	462.17	J/mol×K	677.73	Joback Method
cpg	473.51	J/mol×K	708.58	Joback Method
cpg	484.22	J/mol×K	739.44	Joback Method
cpg	494.33	J/mol×K	770.29	Joback Method
cpg	503.85	J/mol×K	801.15	Joback Method
cpg	512.79	J/mol×K	832.00	Joback Method
dvisc	0.0042998	Pa×s	372.79	Joback Method
dvisc	0.0013868	Pa×s	418.47	Joback Method

dvisc	0.0005589	Pa×s	464.15	Joback Method
dvisc	0.0002650	Pa×s	509.83	Joback Method
dvisc	0.0001421	Pa×s	555.51	Joback Method
dvisc	0.0000838	Pa×s	601.19	Joback Method
dvisc	0.0000532	Pa×s	646.87	Joback Method

Sources

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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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