

Ethylene glycol iso-butyrate-2,2,4-trimethyl-3-oxovalerate

Inchi:	InChI=1S/C14H24O5/c1-9(2)11(15)14(5,6)13(17)19-8-7-18-12(16)10(3)4/h9-10H,7-8H2,
InchiKey:	KHCOOLZMVDKFHC-UHFFFAOYSA-N
Formula:	C14H24O5
SMILES:	CC(C)C(=O)OCCOC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]:	272.34
CAS:	4447-80-7

Physical Properties

Property code	Value	Unit	Source
gf	-531.80	kJ/mol	Joback Method
hf	-953.78	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.980		Crippen Method
mcvol	224.570	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
tb	722.06	K	Joback Method
tc	917.63	K	Joback Method
tf	414.21	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.15	J/molxK	722.06	Joback Method
cpg	662.33	J/molxK	754.65	Joback Method
cpg	676.58	J/molxK	787.25	Joback Method
cpg	689.93	J/molxK	819.84	Joback Method
cpg	702.39	J/molxK	852.44	Joback Method
cpg	713.98	J/molxK	885.03	Joback Method
cpg	724.72	J/molxK	917.63	Joback Method
dvisc	0.0016951	Paxs	414.21	Joback Method
dvisc	0.0007778	Paxs	465.52	Joback Method

dvisc	0.0004166	Paxs	516.83	Joback Method
dvisc	0.0002498	Paxs	568.13	Joback Method
dvisc	0.0001630	Paxs	619.44	Joback Method
dvisc	0.0001135	Paxs	670.75	Joback Method
dvisc	0.0000833	Paxs	722.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4447807&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
mccvol:	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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