2,4,4-Trimethylpentane-1,3-diol diisobutyrate

Inchi: InChI=1S/C15H28O4/c1-9(2)13(19-15(17)11(5)6)12(7)8-18-14(16)10(3)4/h9-13H,8H2,1-
InchiKey: SMGFBRCVKRXTLC-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CC(C)C(=O)OCC(C)C(OC(=O)C(C)C)C(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-404.62	kJ/mol	Joback Method
hf	-868.93	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	3.046		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
ripol	1875.00		NIST Webbook
ripol	1875.00		NIST Webbook
tb	692.98	K	Joback Method
tc	880.79	K	Joback Method
tf	328.13	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.64	J/mol×K	692.98	Joback Method
cpg	696.99	J/mol×K	724.28	Joback Method
cpg	713.41	J/mol×K	755.58	Joback Method
cpg	728.93	J/mol×K	786.88	Joback Method
cpg	743.55	J/mol×K	818.18	Joback Method
cpg	757.27	J/mol×K	849.49	Joback Method
cpg	770.09	J/mol×K	880.79	Joback Method
dvisc	0.0050302	Pa×s	328.13	Joback Method

dvisc	0.0014241	Pa×s	388.94	Joback Method
dvisc	0.0005671	Pa×s	449.75	Joback Method
dvisc	0.0002812	Pa×s	510.56	Joback Method
dvisc	0.0001619	Pa×s	571.36	Joback Method
dvisc	0.0001037	Pa×s	632.17	Joback Method
dvisc	0.0000718	Pa×s	692.98	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R560746&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume