Dimethylmalonic acid, octyl propyl ester

Inchi: InChI=1S/C16H30O4/c1-5-7-8-9-10-11-13-20-15(18)16(3,4)14(17)19-12-6-2/h5-13H2,1-4
InchiKey: UASWFCBSILFDHE-UHFFFAOYSA-N
Formula: C16H30O4
SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)OCCC
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-381.16	kJ/mol	Joback Method
hf	-871.92	kJ/mol	Joback Method
hfus	35.36	kJ/mol	Joback Method
hvap	68.23	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.870		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1753.00		NIST Webbook
tb	714.83	K	Joback Method
tc	896.57	K	Joback Method
tf	416.82	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.69	J/mol×K	714.83	Joback Method
cpg	811.32	J/mol×K	866.28	Joback Method
cpg	797.88	J/mol×K	835.99	Joback Method
cpg	783.62	J/mol×K	805.70	Joback Method
cpg	768.52	J/mol×K	775.41	Joback Method
cpg	752.55	J/mol×K	745.12	Joback Method
cpg	823.95	J/mol×K	896.57	Joback Method
dvisc	0.0000773	Pa×s	714.83	Joback Method
dvisc	0.0001035	Pa×s	665.16	Joback Method

dvisc	0.0001453	Pa×s	615.49	Joback Method
dvisc	0.0002164	Pa×s	565.82	Joback Method
dvisc	0.0003480	Pa×s	516.16	Joback Method
dvisc	0.0006193	Pa×s	466.49	Joback Method
dvisc	0.0012644	Pa×s	416.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361669&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume