

Dimethylmalonic acid, hexyl pentyl ester

Inchi:	InChI=1S/C16H30O4/c1-5-7-9-11-13-20-15(18)16(3,4)14(17)19-12-10-8-6-2/h5-13H2,1-4
InchiKey:	TYIKBCUUIOAULM-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCCCCOC(=O)C(C)(C)C(=O)OCCCCC
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
mvol	251.180	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
tb	714.83	K	Joback Method
tc	896.57	K	Joback Method
tf	416.82	K	Joback Method
vc	0.969	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.69	J/molxK	714.83	Joback Method
cpg	752.55	J/molxK	745.12	Joback Method
cpg	768.52	J/molxK	775.41	Joback Method
cpg	783.62	J/molxK	805.70	Joback Method
cpg	797.88	J/molxK	835.99	Joback Method
cpg	811.32	J/molxK	866.28	Joback Method
cpg	823.95	J/molxK	896.57	Joback Method
dvisc	0.0012644	Paxs	416.82	Joback Method

dvisc	0.0006193	Paxs	466.49	Joback Method
dvisc	0.0003480	Paxs	516.16	Joback Method
dvisc	0.0002164	Paxs	565.82	Joback Method
dvisc	0.0001453	Paxs	615.49	Joback Method
dvisc	0.0001035	Paxs	665.16	Joback Method
dvisc	0.0000773	Paxs	714.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U361686&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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