

Dimethylmalonic acid, hexyl isoheptyl ester

Inchi:	InChI=1S/C17H32O4/c1-6-7-8-9-12-20-15(18)17(4,5)16(19)21-13-10-11-14(2)3/h14H,6-
InchiKey:	ZHYOZGLBYSMTKY-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCCOC(=O)C(C)(C)C(=O)OCCCC(C)C
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-375.18	kJ/mol	Joback Method
hf	-897.84	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.115		Crippen Method
mvol	265.270	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	737.27	K	Joback Method
tc	921.13	K	Joback Method
tf	413.09	K	Joback Method
vc	1.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.34	J/molxK	737.27	Joback Method
cpg	810.75	J/molxK	767.91	Joback Method
cpg	827.21	J/molxK	798.56	Joback Method
cpg	842.74	J/molxK	829.20	Joback Method
cpg	857.37	J/molxK	859.84	Joback Method
cpg	871.12	J/molxK	890.49	Joback Method
cpg	884.02	J/molxK	921.13	Joback Method
dvisc	0.0013901	Paxs	413.09	Joback Method

dvisc	0.0006127	Paxs	467.12	Joback Method
dvisc	0.0003200	Paxs	521.15	Joback Method
dvisc	0.0001889	Paxs	575.18	Joback Method
dvisc	0.0001220	Paxs	629.21	Joback Method
dvisc	0.0000845	Paxs	683.24	Joback Method
dvisc	0.0000617	Paxs	737.27	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=U361687&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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