Dimethylmalonic acid, dihexyl ester

Inchi: InChI=1S/C17H32O4/c1-5-7-9-11-13-20-15(18)17(3,4)16(19)21-14-12-10-8-6-2/h5-14H2
InchiKey: NKWAKHUEIQPPBI-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCCCCCOC(=O)C(C)(C)C(=O)OCCCCCC
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-372.74	kJ/mol	Joback Method
hf	-892.56	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	70.45	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.260		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	1836.00		NIST Webbook
tb	737.71	K	Joback Method
tc	919.59	K	Joback Method
tf	428.09	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.85	J/mol×K	737.71	Joback Method
cpg	869.90	J/mol×K	889.28	Joback Method
cpg	856.24	J/mol×K	858.97	Joback Method
cpg	841.73	J/mol×K	828.65	Joback Method
cpg	826.34	J/mol×K	798.34	Joback Method
cpg	810.06	J/mol×K	768.02	Joback Method
cpg	882.72	J/mol×K	919.59	Joback Method
dvisc	0.0000669	Pa×s	737.71	Joback Method
dvisc	0.0000898	Pa×s	686.11	Joback Method

dvisc	0.0001264	Pa×s	634.50	Joback Method
dvisc	0.0001892	Pa×s	582.90	Joback Method
dvisc	0.0003061	Pa×s	531.30	Joback Method
dvisc	0.0005494	Pa×s	479.69	Joback Method
dvisc	0.0011352	Pa×s	428.09	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=U361688&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