Dimethylmalonic acid, hexyl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C18H32O4/c1-5-6-7-8-13-21-16(19)18(3,4)17(20)22-15-11-9-14(2)10-12-15/h1

InchiKey: KOLBZJZBYUASDY-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-347.58	kJ/mol	Joback Method
hf	-879.22	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	72.80	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.258		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	775.47	K	Joback Method
tc	976.62	K	Joback Method
tf	442.50	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.14	J/mol×K	775.47	Joback Method
cpg	934.51	J/mol×K	943.09	Joback Method
cpg	920.13	J/mol×K	909.57	Joback Method
cpg	904.54	J/mol×K	876.04	Joback Method
cpg	887.69	J/mol×K	842.52	Joback Method
cpg	869.57	J/mol×K	808.99	Joback Method
cpg	947.70	J/mol×K	976.62	Joback Method
dvisc	0.0000751	Pa×s	775.47	Joback Method

dvisc	0.0000998	Pa×s	719.97	Joback Method
dvisc	0.0001390	Pa×s	664.48	Joback Method
dvisc	0.0002057	Pa×s	608.98	Joback Method
dvisc	0.0003294	Pa×s	553.49	Joback Method
dvisc	0.0005858	Pa×s	498.00	Joback Method
dvisc	0.0012035	Pa×s	442.50	Joback Method

Sources

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=U363898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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