Dimethylmalonic acid, isohexyl trans-4-methylcyclohexyl ester

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

InchiKey: GKABQZJQDGTTPN-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-350.02	kJ/mol	Joback Method
hf	-884.50	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	72.41	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.114		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	775.03	K	Joback Method
tc	978.85	K	Joback Method
tf	427.50	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.63	J/mol×K	775.03	Joback Method
cpg	935.87	J/mol×K	944.88	Joback Method
cpg	921.41	J/mol×K	910.91	Joback Method
cpg	905.68	J/mol×K	876.94	Joback Method
cpg	888.66	J/mol×K	842.97	Joback Method
cpg	870.32	J/mol×K	809.00	Joback Method
cpg	949.11	J/mol×K	978.85	Joback Method
dvisc	0.0000691	Pa×s	775.03	Joback Method

dvisc	0.0000935	Pa×s	717.11	Joback Method
dvisc	0.0001333	Pa×s	659.19	Joback Method
dvisc	0.0002035	Pa×s	601.26	Joback Method
dvisc	0.0003402	Pa×s	543.34	Joback Method
dvisc	0.0006426	Pa×s	485.42	Joback Method
dvisc	0.0014425	Pa×s	427.50	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=U363897&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