Dimethylmalonic acid, cis-4-methylcyclohexyl octyl ester

Inchi: InChI=1S/C20H36O4/c1-5-6-7-8-9-10-15-23-18(21)20(3,4)19(22)24-17-13-11-16(2)12-14

InchiKey: HRWBCZRBMZBBHC-UHFFFAOYSA-N

Formula: C20H36O4

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

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-330.74	kJ/mol	Joback Method
hf	-920.50	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.038		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	821.23	K	Joback Method
tc	1021.41	K	Joback Method
tf	465.04	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.35	J/mol×K	821.23	Joback Method
cpg	989.85	J/mol×K	854.59	Joback Method
cpg	1007.99	J/mol×K	887.96	Joback Method
cpg	1024.80	J/mol×K	921.32	Joback Method
cpg	1040.32	J/mol×K	954.68	Joback Method
cpg	1054.58	J/mol×K	988.05	Joback Method
cpg	1067.61	J/mol×K	1021.41	Joback Method
dvisc	0.0009656	Pa×s	465.04	Joback Method

dvisc	0.0004599	Pa×s	524.40	Joback Method
dvisc	0.0002547	Pa×s	583.77	Joback Method
dvisc	0.0001573	Pa×s	643.13	Joback Method
dvisc	0.0001054	Pa×s	702.50	Joback Method
dvisc	0.0000752	Pa×s	761.87	Joback Method
dvisc	0.0000563	Pa×s	821.23	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=U363881&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