

Dimethylmalonic acid, octyl trans-4-methylcyclohexyl 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
mvol	296.680	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2199.00		NIST Webbook
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tb	821.23	K	Joback Method
tc	1021.41	K	Joback Method
tf	465.04	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.35	J/molxK	821.23	Joback Method
cpg	1054.58	J/molxK	988.05	Joback Method
cpg	1040.32	J/molxK	954.68	Joback Method
cpg	1024.80	J/molxK	921.32	Joback Method
cpg	1007.99	J/molxK	887.96	Joback Method
cpg	989.85	J/molxK	854.59	Joback Method
cpg	1067.61	J/molxK	1021.41	Joback Method
dvisc	0.0000563	Paxs	821.23	Joback Method

dvisc	0.0000752	Paxs	761.87	Joback Method
dvisc	0.0001054	Paxs	702.50	Joback Method
dvisc	0.0001573	Paxs	643.13	Joback Method
dvisc	0.0002547	Paxs	583.77	Joback Method
dvisc	0.0004599	Paxs	524.40	Joback Method
dvisc	0.0009656	Paxs	465.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363900&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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