

Dimethylmalonic acid, cis-4-methylcyclohexyl hexyl 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:	CCCCCOC(=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
mvol	268.500	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	775.47	K	Joback Method
tc	976.62	K	Joback Method
tf	442.50	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.14	J/molxK	775.47	Joback Method
cpg	869.57	J/molxK	808.99	Joback Method
cpg	887.69	J/molxK	842.52	Joback Method
cpg	904.54	J/molxK	876.04	Joback Method
cpg	920.13	J/molxK	909.57	Joback Method
cpg	934.51	J/molxK	943.09	Joback Method
cpg	947.70	J/molxK	976.62	Joback Method
dvisc	0.0012035	Paxs	442.50	Joback Method

dvisc	0.0005858	Paxs	498.00	Joback Method
dvisc	0.0003294	Paxs	553.49	Joback Method
dvisc	0.0002057	Paxs	608.98	Joback Method
dvisc	0.0001390	Paxs	664.48	Joback Method
dvisc	0.0000998	Paxs	719.97	Joback Method
dvisc	0.0000751	Paxs	775.47	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=U363879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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

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