

Dimethylmalonic acid, cis-4-methylcyclohexyl pentyl ester

Inchi:	InChI=1S/C17H30O4/c1-5-6-7-12-20-15(18)17(3,4)16(19)21-14-10-8-13(2)9-11-14/h13-1
InchiKey:	JZHWWLWJOWPBOKY-UHFFFAOYSA-N
Formula:	C17H30O4
SMILES:	CCCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-356.00	kJ/mol	Joback Method
hf	-858.58	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	70.57	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.868		Crippen Method
mvol	254.410	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	1951.00		NIST Webbook
rinpol	1951.00		NIST Webbook
tb	752.59	K	Joback Method
tc	955.09	K	Joback Method
tf	431.23	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.27	J/molxK	752.59	Joback Method
cpg	875.57	J/molxK	921.34	Joback Method
cpg	861.17	J/molxK	887.59	Joback Method
cpg	845.57	J/molxK	853.84	Joback Method
cpg	828.74	J/molxK	820.09	Joback Method
cpg	810.64	J/molxK	786.34	Joback Method
cpg	888.80	J/molxK	955.09	Joback Method
dvisc	0.0000864	Paxs	752.59	Joback Method

dvisc	0.0001145	Paxs	699.03	Joback Method
dvisc	0.0001589	Paxs	645.47	Joback Method
dvisc	0.0002342	Paxs	591.91	Joback Method
dvisc	0.0003727	Paxs	538.35	Joback Method
dvisc	0.0006573	Paxs	484.79	Joback Method
dvisc	0.0013348	Paxs	431.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363877&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

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

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