Dimethylmalonic acid, pentyl trans-4-methylcyclohexyl 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: JZHWLWJOWPBOKY-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
mcvol	254.410	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
tb	752.59	K	Joback Method
tc	955.09	K	Joback Method
tf	431.23	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.27	J/mol×K	752.59	Joback Method
cpg	810.64	J/mol×K	786.34	Joback Method
cpg	828.74	J/mol×K	820.09	Joback Method
cpg	845.57	J/mol×K	853.84	Joback Method
cpg	861.17	J/mol×K	887.59	Joback Method
cpg	875.57	J/mol×K	921.34	Joback Method
cpg	888.80	J/mol×K	955.09	Joback Method
dvisc	0.0013348	Pa×s	431.23	Joback Method

dvisc	0.0006573	Pa×s	484.79	Joback Method
dvisc	0.0003727	Pa×s	538.35	Joback Method
dvisc	0.0002342	Pa×s	591.91	Joback Method
dvisc	0.0001589	Pa×s	645.47	Joback Method
dvisc	0.0001145	Pa×s	699.03	Joback Method
dvisc	0.0000864	Pa×s	752.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363896&Units=SI
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

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