Dimethylmalonic acid, 3-methylphenyl pentyl ester

Inchi: InChI=1S/C17H24O4/c1-5-6-7-11-20-15(18)17(3,4)16(19)21-14-10-8-9-13(2)12-14/h8-10

InchiKey: UKQBHTRCKBDOMX-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: CCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-269.96	kJ/mol	Joback Method
hf	-667.50	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.660		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	769.37	K	Joback Method
tc	977.67	K	Joback Method
tf	467.03	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.20	J/mol×K	769.37	Joback Method
cpg	774.31	J/mol×K	942.95	Joback Method
cpg	762.72	J/mol×K	908.23	Joback Method
cpg	750.15	J/mol×K	873.52	Joback Method
cpg	736.56	J/mol×K	838.80	Joback Method
cpg	721.92	J/mol×K	804.09	Joback Method
cpg	784.95	J/mol×K	977.67	Joback Method
dvisc	0.0000668	Pa×s	769.37	Joback Method

dvisc	0.0000867	Pa×s	718.98	Joback Method
dvisc	0.0001172	Pa×s	668.59	Joback Method
dvisc	0.0001663	Pa×s	618.20	Joback Method
dvisc	0.0002511	Pa×s	567.81	Joback Method
dvisc	0.0004108	Pa×s	517.42	Joback Method
dvisc	0.0007474	Pa×s	467.03	Joback Method

Sources

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=U363612&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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