Dimethylmalonic acid, 4-acetylphenyl propyl ester

Inchi: InChI=1S/C16H20O5/c1-5-10-20-14(18)16(3,4)15(19)21-13-8-6-12(7-9-13)11(2)17/h6-9H
InchiKey: ATCKDCIGTISFHB-UHFFFAOYSA-N
Formula: C16H20O5
SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
gf	-407.30	kJ/mol	Joback Method
hf	-759.44	kJ/mol	Joback Method
hfus	30.61	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.774		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2070.00		NIST Webbook
tb	800.36	K	Joback Method
tc	1016.96	K	Joback Method
tf	505.69	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.20	J/mol×K	800.36	Joback Method
cpg	679.88	J/mol×K	836.46	Joback Method
cpg	692.47	J/mol×K	872.56	Joback Method
cpg	704.02	J/mol×K	908.66	Joback Method
cpg	714.54	J/mol×K	944.76	Joback Method
cpg	724.07	J/mol×K	980.86	Joback Method
cpg	732.66	J/mol×K	1016.96	Joback Method
dvisc	0.0006620	Pa×s	505.69	Joback Method
dvisc	0.0003900	Pa×s	554.80	Joback Method

dvisc	0.0002504	Pa×s	603.91	Joback Method
dvisc	0.0001719	Pa×s	653.02	Joback Method
dvisc	0.0001243	Pa×s	702.14	Joback Method
dvisc	0.0000938	Pa×s	751.25	Joback Method
dvisc	0.0000733	Pa×s	800.36	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=U363698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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