Dimethylmalonic acid, 4-acetylphenyl ethyl ester

Inchi: InChI=1S/C15H18O5/c1-5-19-13(17)15(3,4)14(18)20-12-8-6-11(7-9-12)10(2)16/h6-9H,5H

InchiKey: MFTKKTMKNWWZRH-UHFFFAOYSA-N

Formula: C15H18O5

SMILES: CCOC(=O)C(C)(C)C(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 278.30

Physical Properties

Property code	Value	Unit	Source
gf	-415.72	kJ/mol	Joback Method
hf	-738.80	kJ/mol	Joback Method
hfus	28.02	kJ/mol	Joback Method
hvap	75.68	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.384		Crippen Method
mcvol	214.900	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1984.00		NIST Webbook
rinpol	1984.00		NIST Webbook
tb	777.48	K	Joback Method
tc	996.60	K	Joback Method
tf	494.42	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.30	J/mol×K	777.48	Joback Method
cpg	624.71	J/mol×K	814.00	Joback Method
cpg	637.05	J/mol×K	850.52	Joback Method
cpg	648.37	J/mol×K	887.04	Joback Method
cpg	658.68	J/mol×K	923.56	Joback Method
cpg	668.02	J/mol×K	960.08	Joback Method
cpg	676.42	J/mol×K	996.60	Joback Method
dvisc	0.0007284	Pa×s	494.42	Joback Method

dvisc	0.0004348	Pa×s	541.60	Joback Method
dvisc	0.0002820	Pa×s	588.77	Joback Method
dvisc	0.0001950	Pa×s	635.95	Joback Method
dvisc	0.0001419	Pa×s	683.13	Joback Method
dvisc	0.0001075	Pa×s	730.30	Joback Method
dvisc	0.0000843	Pa×s	777.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363697&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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