

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.20	J/molxK	800.36	Joback Method
cpg	724.07	J/molxK	980.86	Joback Method
cpg	714.54	J/molxK	944.76	Joback Method
cpg	704.02	J/molxK	908.66	Joback Method
cpg	692.47	J/molxK	872.56	Joback Method
cpg	679.88	J/molxK	836.46	Joback Method
cpg	732.66	J/molxK	1016.96	Joback Method
dvisc	0.0000733	Paxs	800.36	Joback Method
dvisc	0.0000938	Paxs	751.25	Joback Method

dvisc	0.0001243	Paxs	702.14	Joback Method
dvisc	0.0001719	Paxs	653.02	Joback Method
dvisc	0.0002504	Paxs	603.91	Joback Method
dvisc	0.0003900	Paxs	554.80	Joback Method
dvisc	0.0006620	Paxs	505.69	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.cheméo.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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