Dimethylmalonic acid, di(4-acetylphenyl) ester

Inchi: InChI=1S/C21H20O6/c1-13(22)15-5-9-17(10-6-15)26-19(24)21(3,4)20(25)27-18-11-7-16
InchiKey: ILIGCXNRWFKBSV-UHFFFAOYSA-N
Formula: C21H20O6
SMILES: CC(=O)c1ccc(OC(=O)C(C)(C)C(=O)Oc2ccc(C(C)=O)cc2)cc1
Mol. weight [g/mol]: 368.38

Physical Properties

Property code	Value	Unit	Source
gf	-391.34	kJ/mol	Joback Method
hf	-750.16	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	98.72	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.629		Crippen Method
mcvol	277.250	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2936.00		NIST Webbook
rinpol	2936.00		NIST Webbook
tb	1000.29	K	Joback Method
tc	1243.39	K	Joback Method
tf	650.91	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.23	J/mol×K	1000.29	Joback Method
cpg	864.22	J/mol×K	1040.81	Joback Method
cpg	872.89	J/mol×K	1081.32	Joback Method
cpg	880.30	J/mol×K	1121.84	Joback Method
cpg	886.51	J/mol×K	1162.36	Joback Method
cpg	891.60	J/mol×K	1202.87	Joback Method
cpg	895.64	J/mol×K	1243.39	Joback Method
dvisc	0.0002524	Pa×s	650.91	Joback Method

dvisc	0.0001579	Pa×s	709.14	Joback Method
dvisc	0.0001060	Pa×s	767.37	Joback Method
dvisc	0.0000753	Pa×s	825.60	Joback Method
dvisc	0.0000559	Pa×s	883.83	Joback Method
dvisc	0.0000431	Pa×s	942.06	Joback Method
dvisc	0.0000343	Pa×s	1000.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363711&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