Dimethylmalonic acid, 4-acetylphenyl pentyl ester

Inchi: InChI=1S/C18H24O5/c1-5-6-7-12-22-16(20)18(3,4)17(21)23-15-10-8-14(9-11-15)13(2)19

InchiKey: ISGSDUILHSXYKG-UHFFFAOYSA-N

Formula: C18H24O5

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

Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-390.46	kJ/mol	Joback Method
hf	-800.72	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	82.36	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.554		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2233.00		NIST Webbook
rinpol	2233.00		NIST Webbook
tb	846.12	K	Joback Method
tc	1059.46	K	Joback Method
tf	528.23	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.83	J/mol×K	846.12	Joback Method
cpg	838.41	J/mol×K	1023.90	Joback Method
cpg	828.60	J/mol×K	988.34	Joback Method
cpg	817.77	J/mol×K	952.79	Joback Method
cpg	805.89	J/mol×K	917.23	Joback Method
cpg	792.92	J/mol×K	881.68	Joback Method
cpg	847.24	J/mol×K	1059.46	Joback Method
dvisc	0.0000550	Pa×s	846.12	Joback Method

dvisc	0.0000708	Pa×s	793.14	Joback Method
dvisc	0.0000946	Pa×s	740.16	Joback Method
dvisc	0.0001322	Pa×s	687.17	Joback Method
dvisc	0.0001954	Pa×s	634.19	Joback Method
dvisc	0.0003099	Pa×s	581.21	Joback Method
dvisc	0.0005394	Pa×s	528.23	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=U363699&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