Dimethylmalonic acid, 4-acetylphenyl isohexyl ester

Inchi: InChI=1S/C19H26O5/c1-13(2)7-6-12-23-17(21)19(4,5)18(22)24-16-10-8-15(9-11-16)14(3

InchiKey: FKBOFNHBRWSGEG-UHFFFAOYSA-N

Formula: C19H26O5

SMILES: CC(=O)c1ccc(OC(=O)C(C)(C)C(=O)OCCCC(C)C)cc1

Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-384.48	kJ/mol	Joback Method
hf	-826.64	kJ/mol	Joback Method
hfus	34.85	kJ/mol	Joback Method
hvap	84.20	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.800		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	868.56	K	Joback Method
tc	1083.50	K	Joback Method
tf	524.50	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.94	J/mol×K	868.56	Joback Method
cpg	851.33	J/mol×K	904.38	Joback Method
cpg	864.54	J/mol×K	940.21	Joback Method
cpg	876.60	J/mol×K	976.03	Joback Method
cpg	887.56	J/mol×K	1011.85	Joback Method
cpg	897.45	J/mol×K	1047.67	Joback Method
cpg	906.31	J/mol×K	1083.50	Joback Method
dvisc	0.0005419	Pa×s	524.50	Joback Method

dvisc	0.0002892	Pa×s	581.84	Joback Method
dvisc	0.0001727	Pa×s	639.19	Joback Method
dvisc	0.0001123	Pa×s	696.53	Joback Method
dvisc	0.0000779	Pa×s	753.87	Joback Method
dvisc	0.0000570	Pa×s	811.22	Joback Method
dvisc	0.0000434	Pa×s	868.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363700&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