Diethylmalonic acid, di(4-acetylphenyl) ester

Inchi: InChI=1S/C23H24O6/c1-5-23(6-2,21(26)28-19-11-7-17(8-12-19)15(3)24)22(27)29-20-13-
InchiKey: OARCOSNOWYQPBF-UHFFFAOYSA-N
Formula: C23H24O6
SMILES: CCC(CC)(C(=O)Oc1ccc(C(C)=O)cc1)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 396.43

Physical Properties

Property code	Value	Unit	Source
gf	-374.50	kJ/mol	Joback Method
hf	-791.44	kJ/mol	Joback Method
hfus	43.99	kJ/mol	Joback Method
hvap	103.18	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.409		Crippen Method
mcvol	305.430	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	3195.00		NIST Webbook
rinpol	3195.00		NIST Webbook
tb	1046.05	K	Joback Method
tc	1289.12	K	Joback Method
tf	673.45	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.54	J/mol×K	1046.05	Joback Method
cpg	980.62	J/mol×K	1086.56	Joback Method
cpg	989.36	J/mol×K	1127.07	Joback Method
cpg	996.81	J/mol×K	1167.58	Joback Method
cpg	1003.07	J/mol×K	1208.09	Joback Method
cpg	1008.21	J/mol×K	1248.60	Joback Method
cpg	1012.29	J/mol×K	1289.12	Joback Method
dvisc	0.0001993	Pa×s	673.45	Joback Method

dvisc	0.0001221	Pa×s	735.55	Joback Method
dvisc	0.0000807	Pa×s	797.65	Joback Method
dvisc	0.0000566	Pa×s	859.75	Joback Method
dvisc	0.0000417	Pa×s	921.85	Joback Method
dvisc	0.0000319	Pa×s	983.95	Joback Method
dvisc	0.0000252	Pa×s	1046.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370095&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

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