Diethylmalonic acid, 4-acetylphenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C22H32O5/c1-7-10-19(15(4)5)27-21(25)22(8-2,9-3)20(24)26-18-13-11-17(12-1

InchiKey: WEABGWYQKVSHOG-UHFFFAOYSA-N

Formula: C22H32O5

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1ccc(C(C)=O)cc1)C(C)C

Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-361.66	kJ/mol	Joback Method
hf	-893.84	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	90.49	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.969		Crippen Method
mcvol	313.530	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook
tb	936.76	K	Joback Method
tc	1154.56	K	Joback Method
tf	543.31	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.35	J/mol×K	936.76	Joback Method
cpg	1076.03	J/mol×K	1118.26	Joback Method
cpg	1066.09	J/mol×K	1081.96	Joback Method
cpg	1055.01	J/mol×K	1045.66	Joback Method
cpg	1042.73	J/mol×K	1009.36	Joback Method
cpg	1029.20	J/mol×K	973.06	Joback Method
cpg	1084.87	J/mol×K	1154.56	Joback Method
dvisc	0.0000250	Pa×s	936.76	Joback Method

dvisc	0.0000336	Pa×s	871.18	Joback Method
dvisc	0.0000473	Pa×s	805.61	Joback Method
dvisc	0.0000708	Pa×s	740.03	Joback Method
dvisc	0.0001145	Pa×s	674.46	Joback Method
dvisc	0.0002055	Pa×s	608.88	Joback Method
dvisc	0.0004248	Pa×s	543.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370083&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