Diethylmalonic acid, 4-acetylphenyl heptyl ester

Inchi: InChI=1S/C22H32O5/c1-5-8-9-10-11-16-26-20(24)22(6-2,7-3)21(25)27-19-14-12-18(13-1

InchiKey: SQLZEAAQSFKMSM-UHFFFAOYSA-N

Formula: C22H32O5

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-356.78	kJ/mol	Joback Method
hf	-883.28	kJ/mol	Joback Method
hfus	46.15	kJ/mol	Joback Method
hvap	91.27	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.115		Crippen Method
mcvol	313.530	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2610.00		NIST Webbook
rinpol	2610.00		NIST Webbook
tb	937.64	K	Joback Method
tc	1152.88	K	Joback Method
tf	573.31	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.44	J/mol×K	937.64	Joback Method
cpg	1075.22	J/mol×K	1117.01	Joback Method
cpg	1065.16	J/mol×K	1081.13	Joback Method
cpg	1054.01	J/mol×K	1045.26	Joback Method
cpg	1041.70	J/mol×K	1009.39	Joback Method
cpg	1028.20	J/mol×K	973.51	Joback Method
cpg	1084.23	J/mol×K	1152.88	Joback Method
dvisc	0.0000301	Pa×s	937.64	Joback Method

dvisc	0.0000392	Pa×s	876.92	Joback Method
dvisc	0.0000531	Pa×s	816.20	Joback Method
dvisc	0.0000756	Pa×s	755.47	Joback Method
dvisc	0.0001145	Pa×s	694.75	Joback Method
dvisc	0.0001878	Pa×s	634.03	Joback Method
dvisc	0.0003420	Pa×s	573.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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