Diethylmalonic acid, 4-acetylphenyl dodecyl ester

Inchi: InChI=1S/C27H42O5/c1-5-8-9-10-11-12-13-14-15-16-21-31-25(29)27(6-2,7-3)26(30)32-2
InchiKey: YYCLABQHGLIJLC-UHFFFAOYSA-N
Formula: C27H42O5
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 446.62

Physical Properties

Property code	Value	Unit	Source
gf	-314.68	kJ/mol	Joback Method
hf	-986.48	kJ/mol	Joback Method
hfus	59.10	kJ/mol	Joback Method
hvap	102.40	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.065		Crippen Method
mcvol	383.980	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	1052.04	K	Joback Method
tc	1289.96	K	Joback Method
tf	629.66	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.61	J/mol×K	1052.04	Joback Method
cpg	1335.49	J/mol×K	1091.69	Joback Method
cpg	1349.81	J/mol×K	1131.35	Joback Method
cpg	1362.65	J/mol×K	1171.00	Joback Method
cpg	1374.11	J/mol×K	1210.65	Joback Method
cpg	1384.28	J/mol×K	1250.31	Joback Method
cpg	1393.26	J/mol×K	1289.96	Joback Method
dvisc	0.0001810	Pa×s	629.66	Joback Method

dvisc	0.0000947	Pa×s	700.06	Joback Method
dvisc	0.0000557	Pa×s	770.45	Joback Method
dvisc	0.0000359	Pa×s	840.85	Joback Method
dvisc	0.0000247	Pa×s	911.25	Joback Method
dvisc	0.0000179	Pa×s	981.64	Joback Method
dvisc	0.0000136	Pa×s	1052.04	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=U370090&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