Diethylmalonic acid, 4-acetylphenyl tetradecyl ester

Inchi: InChI=1S/C29H46O5/c1-5-8-9-10-11-12-13-14-15-16-17-18-23-33-27(31)29(6-2,7-3)28(3

InchiKey: CSRZYSLGEUIUJQ-UHFFFAOYSA-N

Formula: C29H46O5

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

Mol. weight [g/mol]: 474.67

Physical Properties

Property code	Value	Unit	Source
gf	-297.84	kJ/mol	Joback Method
hf	-1027.76	kJ/mol	Joback Method
hfus	64.28	kJ/mol	Joback Method
hvap	106.85	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	7.845		Crippen Method
mcvol	412.160	ml/mol	McGowan Method
pc	810.76	kPa	Joback Method
rinpol	3315.00		NIST Webbook
rinpol	3315.00		NIST Webbook
tb	1097.80	K	Joback Method
tc	1352.87	K	Joback Method
tf	652.20	K	Joback Method
vc	1.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1444.93	J/mol×K	1097.80	Joback Method
cpg	1461.49	J/mol×K	1140.31	Joback Method
cpg	1476.29	J/mol×K	1182.82	Joback Method
cpg	1489.45	J/mol×K	1225.33	Joback Method
cpg	1501.08	J/mol×K	1267.84	Joback Method
cpg	1511.32	J/mol×K	1310.35	Joback Method
cpg	1520.29	J/mol×K	1352.87	Joback Method
dvisc	0.0001380	Pa×s	652.20	Joback Method

dvisc	0.0000709	Pa×s	726.47	Joback Method
dvisc	0.0000412	Pa×s	800.73	Joback Method
dvisc	0.0000263	Pa×s	875.00	Joback Method
dvisc	0.0000180	Pa×s	949.27	Joback Method
dvisc	0.0000130	Pa×s	1023.53	Joback Method
dvisc	0.0000098	Pa×s	1097.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370092&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