Diethylmalonic acid, 4-acetylphenyl hexadecyl ester

Inchi: InChI=1S/C31H50O5/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-25-35-29(33)31(6-2,7-

InchiKey: MOGLNYBTKDWRNS-UHFFFAOYSA-N

Formula: C31H50O5

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

Mol. weight [g/mol]: 502.73

Physical Properties

Property code	Value	Unit	Source
gf	-281.00	kJ/mol	Joback Method
hf	-1069.04	kJ/mol	Joback Method
hfus	69.46	kJ/mol	Joback Method
hvap	111.30	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	8.626		Crippen Method
mcvol	440.340	ml/mol	McGowan Method
pc	728.88	kPa	Joback Method
rinpol	3537.00		NIST Webbook
rinpol	3537.00		NIST Webbook
tb	1143.56	K	Joback Method
tc	1421.44	K	Joback Method
tf	674.74	K	Joback Method
vc	1.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1571.45	J/mol×K	1143.56	Joback Method
cpg	1588.90	J/mol×K	1189.87	Joback Method
cpg	1604.31	J/mol×K	1236.19	Joback Method
cpg	1617.87	J/mol×K	1282.50	Joback Method
cpg	1629.75	J/mol×K	1328.81	Joback Method
cpg	1640.13	J/mol×K	1375.13	Joback Method
cpg	1649.18	J/mol×K	1421.44	Joback Method
dvisc	0.0001044	Pa×s	674.74	Joback Method

dvisc	0.0000528	Pa×s	752.88	Joback Method
dvisc	0.0000303	Pa×s	831.01	Joback Method
dvisc	0.0000192	Pa×s	909.15	Joback Method
dvisc	0.0000130	Pa×s	987.29	Joback Method
dvisc	0.0000094	Pa×s	1065.42	Joback Method
dvisc	0.0000071	Pa×s	1143.56	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=U370094&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