Diethylmalonic acid, 4-acetylphenyl decyl ester

Inchi: InChI=1S/C25H38O5/c1-5-8-9-10-11-12-13-14-19-29-23(27)25(6-2,7-3)24(28)30-22-17-1

InchiKey: VBBQVPKZDPNAKQ-UHFFFAOYSA-N

Formula: C25H38O5

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

Mol. weight [g/mol]: 418.57

Physical Properties

Property code	Value	Unit	Source
gf	-331.52	kJ/mol	Joback Method
hf	-945.20	kJ/mol	Joback Method
hfus	53.92	kJ/mol	Joback Method
hvap	97.94	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.285		Crippen Method
mcvol	355.800	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	2909.00		NIST Webbook
tb	1006.28	K	Joback Method
tc	1231.98	K	Joback Method
tf	607.12	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.77	J/mol×K	1006.28	Joback Method
cpg	1259.11	J/mol×K	1194.36	Joback Method
cpg	1248.98	J/mol×K	1156.75	Joback Method
cpg	1237.65	J/mol×K	1119.13	Joback Method
cpg	1225.05	J/mol×K	1081.51	Joback Method
cpg	1211.11	J/mol×K	1043.90	Joback Method
cpg	1268.11	J/mol×K	1231.98	Joback Method
dvisc	0.0000188	Pa×s	1006.28	Joback Method
dvisc	0.0000246	Pa×s	939.75	Joback Method

dvisc	0.0000337	Pa×s	873.23	Joback Method
dvisc	0.0000486	Pa×s	806.70	Joback Method
dvisc	0.0000748	Pa×s	740.17	Joback Method
dvisc	0.0001253	Pa×s	673.65	Joback Method
dvisc	0.0002352	Pa×s	607.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370088&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

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