Diethylmalonic acid, 4-biphenyl dodecyl ester

Inchi: InChI=1S/C31H44O4/c1-4-7-8-9-10-11-12-13-14-18-25-34-29(32)31(5-2,6-3)30(33)35-28
InchiKey: XXJQSYLCLBXJJI-UHFFFAOYSA-N
Formula: C31H44O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 480.68

Physical Properties

Property code	Value	Unit	Source
gf	-39.67	kJ/mol	Joback Method
hf	-719.93	kJ/mol	Joback Method
hfus	61.90	kJ/mol	Joback Method
hvap	106.83	kJ/mol	Joback Method
log10ws	-10.13		Crippen Method
logp	8.530		Crippen Method
mcvol	415.010	ml/mol	McGowan Method
pc	847.02	kPa	Joback Method
rinpol	3509.00		NIST Webbook
rinpol	3509.00		NIST Webbook
tb	1116.37	K	Joback Method
tc	1369.23	K	Joback Method
tf	651.23	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1447.95	J/mol×K	1116.37	Joback Method
cpg	1513.35	J/mol×K	1327.09	Joback Method
cpg	1502.74	J/mol×K	1284.95	Joback Method
cpg	1491.04	J/mol×K	1242.80	Joback Method
cpg	1478.11	J/mol×K	1200.66	Joback Method
cpg	1463.80	J/mol×K	1158.51	Joback Method
cpg	1523.02	J/mol×K	1369.23	Joback Method
dvisc	0.0000080	Pa×s	1116.37	Joback Method

dvisc	0.0000106	Pa×s	1038.85	Joback Method
dvisc	0.0000147	Pa×s	961.32	Joback Method
dvisc	0.0000216	Pa×s	883.80	Joback Method
dvisc	0.0000343	Pa×s	806.28	Joback Method
dvisc	0.0000598	Pa×s	728.75	Joback Method
dvisc	0.0001192	Pa×s	651.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370432&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