Diethylmalonic acid, 4-biphenyl undecyl ester

Inchi: InChI=1S/C30H42O4/c1-4-7-8-9-10-11-12-13-17-24-33-28(31)30(5-2,6-3)29(32)34-27-22
InchiKey: UJLOIQCTYHXFCN-UHFFFAOYSA-N
Formula: C30H42O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 466.65

Physical Properties

Property code	Value	Unit	Source
gf	-48.09	kJ/mol	Joback Method
hf	-699.29	kJ/mol	Joback Method
hfus	59.31	kJ/mol	Joback Method
hvap	104.60	kJ/mol	Joback Method
log10ws	-9.71		Crippen Method
logp	8.139		Crippen Method
mcvol	400.920	ml/mol	McGowan Method
pc	896.41	kPa	Joback Method
rinpol	3395.00		NIST Webbook
rinpol	3395.00		NIST Webbook
tb	1093.49	K	Joback Method
tc	1339.37	K	Joback Method
tf	639.96	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1385.18	J/mol×K	1093.49	Joback Method
cpg	1449.45	J/mol×K	1298.39	Joback Method
cpg	1439.03	J/mol×K	1257.41	Joback Method
cpg	1427.52	J/mol×K	1216.43	Joback Method
cpg	1414.80	J/mol×K	1175.45	Joback Method
cpg	1400.73	J/mol×K	1134.47	Joback Method
cpg	1458.92	J/mol×K	1339.37	Joback Method
dvisc	0.0000094	Pa×s	1093.49	Joback Method

dvisc	0.0000125	Pa×s	1017.90	Joback Method
dvisc	0.0000172	Pa×s	942.31	Joback Method
dvisc	0.0000253	Pa×s	866.73	Joback Method
dvisc	0.0000398	Pa×s	791.14	Joback Method
dvisc	0.0000691	Pa×s	715.55	Joback Method
dvisc	0.0001366	Pa×s	639.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370431&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