Diethylmalonic acid, 4-biphenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C26H34O4/c1-6-12-23(19(4)5)30-25(28)26(7-2,8-3)24(27)29-22-17-15-21(16-1

InchiKey: LCOSHVHLSONIBS-UHFFFAOYSA-N

Formula: C26H34O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1)C(C)C

Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-86.65	kJ/mol	Joback Method
hf	-627.29	kJ/mol	Joback Method
hfus	41.90	kJ/mol	Joback Method
hvap	94.92	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.433		Crippen Method
mcvol	344.560	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2885.00		NIST Webbook
tb	1001.09	K	Joback Method
tc	1233.14	K	Joback Method
tf	564.88	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1138.62	J/mol×K	1001.09	Joback Method
cpg	1199.89	J/mol×K	1194.46	Joback Method
cpg	1190.08	J/mol×K	1155.79	Joback Method
cpg	1179.14	J/mol×K	1117.11	Joback Method
cpg	1166.98	J/mol×K	1078.44	Joback Method
cpg	1153.51	J/mol×K	1039.76	Joback Method
cpg	1208.66	J/mol×K	1233.14	Joback Method
dvisc	0.0000147	Pa×s	1001.09	Joback Method
dvisc	0.0000199	Pa×s	928.39	Joback Method

dvisc	0.0000282	Pa×s	855.69	Joback Method
dvisc	0.0000427	Pa×s	782.98	Joback Method
dvisc	0.0000704	Pa×s	710.28	Joback Method
dvisc	0.0001302	Pa×s	637.58	Joback Method
dvisc	0.0002820	Pa×s	564.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370425&Units=SI

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