Diethylmalonic acid, 4-biphenyl heptyl ester

Inchi: InChI=1S/C26H34O4/c1-4-7-8-9-13-20-29-24(27)26(5-2,6-3)25(28)30-23-18-16-22(17-19
InchiKey: DQDHEKWWONYPEK-UHFFFAOYSA-N
Formula: C26H34O4
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-81.77	kJ/mol	Joback Method
hf	-616.73	kJ/mol	Joback Method
hfus	48.95	kJ/mol	Joback Method
hvap	95.70	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	6.579		Crippen Method
mcvol	344.560	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
rinpol	3021.00		NIST Webbook
tb	1001.97	K	Joback Method
tc	1231.42	K	Joback Method
tf	594.88	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.91	J/mol×K	1001.97	Joback Method
cpg	1199.62	J/mol×K	1193.18	Joback Method
cpg	1189.62	J/mol×K	1154.94	Joback Method
cpg	1178.53	J/mol×K	1116.70	Joback Method
cpg	1166.28	J/mol×K	1078.45	Joback Method
cpg	1152.77	J/mol×K	1040.21	Joback Method
cpg	1208.65	J/mol×K	1231.42	Joback Method
dvisc	0.0000178	Pa×s	1001.97	Joback Method
dvisc	0.0000234	Pa×s	934.12	Joback Method

dvisc	0.0000320	Pa×s	866.27	Joback Method
dvisc	0.0000462	Pa×s	798.42	Joback Method
dvisc	0.0000715	Pa×s	730.58	Joback Method
dvisc	0.0001209	Pa×s	662.73	Joback Method
dvisc	0.0002307	Pa×s	594.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370427&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