Diethylmalonic acid, 2,3-dimethylphenyl pentadecyl ester

Inchi: InChI=1S/C30H50O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-24-33-28(31)30(7-2,8-3)
InchiKey: LSNAVAHTRIMYLA-UHFFFAOYSA-N
Formula: C30H50O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-170.13	kJ/mol	Joback Method
hf	-947.29	kJ/mol	Joback Method
hfus	64.88	kJ/mol	Joback Method
hvap	102.99	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.650		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	736.02	kPa	Joback Method
rinpol	3217.00		NIST Webbook
tb	1071.79	K	Joback Method
tc	1321.08	K	Joback Method
tf	626.06	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.14	J/mol×K	1071.79	Joback Method
cpg	1573.12	J/mol×K	1279.53	Joback Method
cpg	1560.93	J/mol×K	1237.98	Joback Method
cpg	1547.25	J/mol×K	1196.43	Joback Method
cpg	1531.97	J/mol×K	1154.89	Joback Method
cpg	1514.97	J/mol×K	1113.34	Joback Method
cpg	1583.94	J/mol×K	1321.08	Joback Method
dvisc	0.0000093	Pa×s	1071.79	Joback Method
dvisc	0.0000124	Pa×s	997.50	Joback Method

dvisc	0.0000171	Pa×s	923.21	Joback Method
dvisc	0.0000252	Pa×s	848.92	Joback Method
dvisc	0.0000397	Pa×s	774.64	Joback Method
dvisc	0.0000691	Pa×s	700.35	Joback Method
dvisc	0.0001371	Pa×s	626.06	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370576&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