Diethylmalonic acid, 2,3-dimethylphenyl dodecyl ester

Inchi: InChI=1S/C27H44O4/c1-6-9-10-11-12-13-14-15-16-17-21-30-25(28)27(7-2,8-3)26(29)31-
InchiKey: PGBOPQDIQHZDSI-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-195.39	kJ/mol	Joback Method
hf	-885.37	kJ/mol	Joback Method
hfus	57.11	kJ/mol	Joback Method
hvap	96.31	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.479		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	866.07	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	1003.15	K	Joback Method
tc	1228.60	K	Joback Method
tf	592.25	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.74	J/mol×K	1003.15	Joback Method
cpg	1323.44	J/mol×K	1040.72	Joback Method
cpg	1339.62	J/mol×K	1078.30	Joback Method
cpg	1354.37	J/mol×K	1115.87	Joback Method
cpg	1367.74	J/mol×K	1153.45	Joback Method
cpg	1379.83	J/mol×K	1191.02	Joback Method
cpg	1390.69	J/mol×K	1228.60	Joback Method
dvisc	0.0002036	Pa×s	592.25	Joback Method

dvisc	0.0001054	Pa×s	660.73	Joback Method
dvisc	0.0000618	Pa×s	729.22	Joback Method
dvisc	0.0000397	Pa×s	797.70	Joback Method
dvisc	0.0000273	Pa×s	866.18	Joback Method
dvisc	0.0000199	Pa×s	934.67	Joback Method
dvisc	0.0000151	Pa×s	1003.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370573&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