Diethylmalonic acid, 2,3-dimethylphenyl tridecyl ester

Inchi: InChI=1S/C28H46O4/c1-6-9-10-11-12-13-14-15-16-17-18-22-31-26(29)28(7-2,8-3)27(30)
InchiKey: RYTWXOWMMFNORR-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-186.97	kJ/mol	Joback Method
hf	-906.01	kJ/mol	Joback Method
hfus	59.70	kJ/mol	Joback Method
hvap	98.54	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	7.869		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	819.13	kPa	Joback Method
rinpol	3014.00		NIST Webbook
tb	1026.03	K	Joback Method
tc	1258.19	K	Joback Method
tf	603.52	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1368.85	J/mol×K	1026.03	Joback Method
cpg	1443.79	J/mol×K	1219.50	Joback Method
cpg	1431.67	J/mol×K	1180.80	Joback Method
cpg	1418.21	J/mol×K	1142.11	Joback Method
cpg	1403.30	J/mol×K	1103.42	Joback Method
cpg	1386.88	J/mol×K	1064.72	Joback Method
cpg	1454.63	J/mol×K	1258.19	Joback Method
dvisc	0.0000129	Pa×s	1026.03	Joback Method
dvisc	0.0000170	Pa×s	955.61	Joback Method

dvisc	0.0000234	Pa×s	885.19	Joback Method
dvisc	0.0000341	Pa×s	814.77	Joback Method
dvisc	0.0000534	Pa×s	744.36	Joback Method
dvisc	0.0000918	Pa×s	673.94	Joback Method
dvisc	0.0001789	Pa×s	603.52	Joback Method

Sources

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=U370574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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