Diethylmalonic acid, 2,3-dimethylphenyl undecyl ester

Inchi: InChI=1S/C26H42O4/c1-6-9-10-11-12-13-14-15-16-20-29-24(27)26(7-2,8-3)25(28)30-23-
InchiKey: WVIWDLBDAKELMR-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-203.81	kJ/mol	Joback Method
hf	-864.73	kJ/mol	Joback Method
hfus	54.52	kJ/mol	Joback Method
hvap	94.09	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.089		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	980.27	K	Joback Method
tc	1200.13	K	Joback Method
tf	580.98	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.04	J/mol×K	980.27	Joback Method
cpg	1316.37	J/mol×K	1163.49	Joback Method
cpg	1304.32	J/mol×K	1126.84	Joback Method
cpg	1291.02	J/mol×K	1090.20	Joback Method
cpg	1276.42	J/mol×K	1053.56	Joback Method
cpg	1260.45	J/mol×K	1016.91	Joback Method
cpg	1327.25	J/mol×K	1200.13	Joback Method
dvisc	0.0000177	Pa×s	980.27	Joback Method

dvisc	0.0000232	Pa×s	913.72	Joback Method
dvisc	0.0000318	Pa×s	847.17	Joback Method
dvisc	0.0000460	Pa×s	780.62	Joback Method
dvisc	0.0000713	Pa×s	714.08	Joback Method
dvisc	0.0001209	Pa×s	647.53	Joback Method
dvisc	0.0002313	Pa×s	580.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370572&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