Diethylmalonic acid, decyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C25H40O4/c1-6-9-10-11-12-13-14-15-19-28-23(26)25(7-2,8-3)24(27)29-22-18-
InchiKey: AXCWBBCHOCIEPI-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-212.23	kJ/mol	Joback Method
hf	-844.09	kJ/mol	Joback Method
hfus	51.93	kJ/mol	Joback Method
hvap	91.86	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.699		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
rinpol	2690.00		NIST Webbook
tb	957.39	K	Joback Method
tc	1172.71	K	Joback Method
tf	569.71	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.78	J/mol×K	957.39	Joback Method
cpg	1253.45	J/mol×K	1136.82	Joback Method
cpg	1241.43	J/mol×K	1100.93	Joback Method
cpg	1228.20	J/mol×K	1065.05	Joback Method
cpg	1213.73	J/mol×K	1029.16	Joback Method
cpg	1197.94	J/mol×K	993.28	Joback Method
cpg	1264.34	J/mol×K	1172.71	Joback Method
dvisc	0.0000207	Pa×s	957.39	Joback Method
dvisc	0.0000271	Pa×s	892.78	Joback Method

dvisc	0.0000370	Pa×s	828.16	Joback Method
dvisc	0.0000533	Pa×s	763.55	Joback Method
dvisc	0.0000822	Pa×s	698.94	Joback Method
dvisc	0.0001383	Pa×s	634.32	Joback Method
dvisc	0.0002619	Pa×s	569.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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