Diethylmalonic acid, decyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C25H40O6/c1-6-9-10-11-12-13-14-15-19-30-23(26)25(7-2,8-3)24(27)31-22-20

InchiKey: PXKVTKQEGFMWKV-UHFFFAOYSA-N

Formula: C25H40O6

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 436.58

Physical Properties

Property code	Value	Unit	Source
gf	-422.23	kJ/mol	Joback Method
hf	-1108.53	kJ/mol	Joback Method
hfus	54.30	kJ/mol	Joback Method
hvap	96.68	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.099		Crippen Method
mcvol	365.970	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tb	1002.23	K	Joback Method
tc	1227.28	K	Joback Method
tf	614.17	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.98	J/mol×K	1002.23	Joback Method
cpg	1254.51	J/mol×K	1039.74	Joback Method
cpg	1268.28	J/mol×K	1077.25	Joback Method
cpg	1280.34	J/mol×K	1114.75	Joback Method
cpg	1290.71	J/mol×K	1152.26	Joback Method
cpg	1299.41	J/mol×K	1189.77	Joback Method
cpg	1306.49	J/mol×K	1227.28	Joback Method
dvisc	0.0001234	Pa×s	614.17	Joback Method

dvisc	0.0000683	Pa×s	678.85	Joback Method
dvisc	0.0000419	Pa×s	743.52	Joback Method
dvisc	0.0000278	Pa×s	808.20	Joback Method
dvisc	0.0000196	Pa×s	872.88	Joback Method
dvisc	0.0000145	Pa×s	937.55	Joback Method
dvisc	0.0000111	Pa×s	1002.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369817&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