Diethylmalonic acid, 2,6-dimethoxyphenyl hexyl ester

Inchi: InChI=1S/C21H32O6/c1-6-9-10-11-15-26-19(22)21(7-2,8-3)20(23)27-18-16(24-4)13-12-1

InchiKey: SDKCPEGTXPMWRU-UHFFFAOYSA-N

Formula: C21H32O6

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

Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
gf	-455.91	kJ/mol	Joback Method
hf	-1025.97	kJ/mol	Joback Method
hfus	43.94	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.539		Crippen Method
mcvol	309.610	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	2489.00		NIST Webbook
rinpol	2489.00		NIST Webbook
tb	910.71	K	Joback Method
tc	1120.29	K	Joback Method
tf	569.09	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.64	J/mol×K	910.71	Joback Method
cpg	1010.80	J/mol×K	945.64	Joback Method
cpg	1024.57	J/mol×K	980.57	Joback Method
cpg	1036.97	J/mol×K	1015.50	Joback Method
cpg	1048.01	J/mol×K	1050.43	Joback Method
cpg	1057.71	J/mol×K	1085.36	Joback Method
cpg	1066.07	J/mol×K	1120.29	Joback Method
dvisc	0.0002013	Pa×s	569.09	Joback Method

dvisc	0.0001162	Pa×s	626.03	Joback Method
dvisc	0.0000735	Pa×s	682.96	Joback Method
dvisc	0.0000499	Pa×s	739.90	Joback Method
dvisc	0.0000358	Pa×s	796.84	Joback Method
dvisc	0.0000268	Pa×s	853.77	Joback Method
dvisc	0.0000208	Pa×s	910.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369813&Units=SI

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

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