Diethylmalonic acid, 2,6-dimethoxyphenyl pentyl ester

Inchi: InChI=1S/C20H30O6/c1-6-9-10-14-25-18(21)20(7-2,8-3)19(22)26-17-15(23-4)12-11-13-1

InchiKey: QOOKLABLLUOCSD-UHFFFAOYSA-N

Formula: C20H30O6

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

Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
gf	-464.33	kJ/mol	Joback Method
hf	-1005.33	kJ/mol	Joback Method
hfus	41.35	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.149		Crippen Method
mcvol	295.520	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2396.00		NIST Webbook
tb	887.83	K	Joback Method
tc	1095.80	K	Joback Method
tf	557.82	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.08	J/mol×K	887.83	Joback Method
cpg	951.13	J/mol×K	922.49	Joback Method
cpg	964.87	J/mol×K	957.15	Joback Method
cpg	977.30	J/mol×K	991.81	Joback Method
cpg	988.43	J/mol×K	1026.48	Joback Method
cpg	998.27	J/mol×K	1061.14	Joback Method
cpg	1006.82	J/mol×K	1095.80	Joback Method
dvisc	0.0002257	Pa×s	557.82	Joback Method
dvisc	0.0001318	Pa×s	612.82	Joback Method

dvisc	0.0000841	Pa×s	667.82	Joback Method
dvisc	0.0000574	Pa×s	722.82	Joback Method
dvisc	0.0000414	Pa×s	777.83	Joback Method
dvisc	0.0000311	Pa×s	832.83	Joback Method
dvisc	0.0000243	Pa×s	887.83	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=U369812&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