Diethylmalonic acid, 2,6-dimethoxyphenyl ethyl ester

Inchi: InChI=1S/C17H24O6/c1-6-17(7-2,15(18)22-8-3)16(19)23-14-12(20-4)10-9-11-13(14)21-5

InchiKey: ISFGXUHZZGGZKG-UHFFFAOYSA-N

Formula: C17H24O6

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

Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-489.59	kJ/mol	Joback Method
hf	-943.41	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.979		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	819.19	K	Joback Method
tc	1026.82	K	Joback Method
tf	524.01	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.48	J/mol×K	819.19	Joback Method
cpg	776.14	J/mol×K	853.80	Joback Method
cpg	789.64	J/mol×K	888.40	Joback Method
cpg	801.98	J/mol×K	923.01	Joback Method
cpg	813.16	J/mol×K	957.61	Joback Method
cpg	823.18	J/mol×K	992.22	Joback Method
cpg	832.04	J/mol×K	1026.82	Joback Method
dvisc	0.0003118	Pa×s	524.01	Joback Method

dvisc	0.0001888	Pa×s	573.21	Joback Method
dvisc	0.0001237	Pa×s	622.40	Joback Method
dvisc	0.0000863	Pa×s	671.60	Joback Method
dvisc	0.0000632	Pa×s	720.80	Joback Method
dvisc	0.0000482	Pa×s	769.99	Joback Method
dvisc	0.0000379	Pa×s	819.19	Joback Method

Sources

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=U369809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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