Diethylmalonic acid, di(2,6-dimethoxyphenyl) ester

Inchi: InChI=1S/C23H28O8/c1-7-23(8-2,21(24)30-19-15(26-3)11-9-12-16(19)27-4)22(25)31-20-
InchiKey: WHCVATGOQAVFTQ-UHFFFAOYSA-N
Formula: C23H28O8
SMILES: CCC(CC)(C(=O)Oc1c(OC)cccc1OC)C(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 432.46

Physical Properties

Property code	Value	Unit	Source
gf	-555.92	kJ/mol	Joback Method
hf	-1118.10	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	100.65	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.038		Crippen Method
mcvol	325.770	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2963.00		NIST Webbook
rinpol	2963.00		NIST Webbook
tb	1037.95	K	Joback Method
tc	1273.44	K	Joback Method
tf	687.55	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.40	J/mol×K	1037.95	Joback Method
cpg	1067.91	J/mol×K	1077.20	Joback Method
cpg	1075.30	J/mol×K	1116.45	Joback Method
cpg	1080.55	J/mol×K	1155.70	Joback Method
cpg	1083.63	J/mol×K	1194.94	Joback Method
cpg	1084.54	J/mol×K	1234.19	Joback Method
cpg	1083.23	J/mol×K	1273.44	Joback Method
dvisc	0.0000576	Pa×s	687.55	Joback Method

dvisc	0.0000374	Pa×s	745.95	Joback Method
dvisc	0.0000258	Pa×s	804.35	Joback Method
dvisc	0.0000187	Pa×s	862.75	Joback Method
dvisc	0.0000142	Pa×s	921.15	Joback Method
dvisc	0.0000111	Pa×s	979.55	Joback Method
dvisc	0.0000089	Pa×s	1037.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369818&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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