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

Inchi: InChI=1S/C21H24O8/c1-21(2,19(22)28-17-13(24-3)9-7-10-14(17)25-4)20(23)29-18-15(2

InchiKey: YOWLGKYNJLXXEY-UHFFFAOYSA-N

Formula: C21H24O8

SMILES: COc1cccc(OC)c1OC(=O)C(C)(C)C(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 404.41

Physical Properties

Property code	Value	Unit	Source
gf	-572.76	kJ/mol	Joback Method
hf	-1076.82	kJ/mol	Joback Method
hfus	39.58	kJ/mol	Joback Method
hvap	96.20	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.258		Crippen Method
mcvol	297.590	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2776.00		NIST Webbook
rinpol	2776.00		NIST Webbook
tb	992.19	K	Joback Method
tc	1224.17	K	Joback Method
tf	665.01	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.83	J/mol×K	992.19	Joback Method
cpg	951.96	J/mol×K	1030.85	Joback Method
cpg	960.16	J/mol×K	1069.52	Joback Method
cpg	966.40	J/mol×K	1108.18	Joback Method
cpg	970.67	J/mol×K	1146.84	Joback Method
cpg	972.92	J/mol×K	1185.50	Joback Method
cpg	973.12	J/mol×K	1224.17	Joback Method
dvisc	0.0000729	Pa×s	665.01	Joback Method

dvisc	0.0000483	Pa×s	719.54	Joback Method
dvisc	0.0000339	Pa×s	774.07	Joback Method
dvisc	0.0000249	Pa×s	828.60	Joback Method
dvisc	0.0000190	Pa×s	883.13	Joback Method
dvisc	0.0000150	Pa×s	937.66	Joback Method
dvisc	0.0000121	Pa×s	992.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363629&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