Diethylmalonic acid, 2,6-dimethoxyphenyl propyl ester

Inchi: InChI=1S/C18H26O6/c1-6-12-23-16(19)18(7-2,8-3)17(20)24-15-13(21-4)10-9-11-14(15)2

InchiKey: CDISSMTXBVARLY-UHFFFAOYSA-N

Formula: C18H26O6

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

Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-481.17	kJ/mol	Joback Method
hf	-964.05	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.369		Crippen Method
mcvol	267.340	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	2225.00		NIST Webbook
tb	842.07	K	Joback Method
tc	1049.12	K	Joback Method
tf	535.28	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.92	J/mol×K	842.07	Joback Method
cpg	880.95	J/mol×K	1014.61	Joback Method
cpg	870.95	J/mol×K	980.10	Joback Method
cpg	859.75	J/mol×K	945.59	Joback Method
cpg	847.35	J/mol×K	911.09	Joback Method
cpg	833.74	J/mol×K	876.58	Joback Method
cpg	889.76	J/mol×K	1049.12	Joback Method
dvisc	0.0000328	Pa×s	842.07	Joback Method
dvisc	0.0000418	Pa×s	790.94	Joback Method

dvisc	0.0000550	Pa×s	739.81	Joback Method
dvisc	0.0000755	Pa×s	688.67	Joback Method
dvisc	0.0001091	Pa×s	637.54	Joback Method
dvisc	0.0001680	Pa×s	586.41	Joback Method
dvisc	0.0002810	Pa×s	535.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369810&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