Diethylmalonic acid, 2,6-dimethoxyphenyl octyl ester

Inchi: InChI=1S/C23H36O6/c1-6-9-10-11-12-13-17-28-21(24)23(7-2,8-3)22(25)29-20-18(26-4)1

InchiKey: WUOYBYKNCCKQQV-UHFFFAOYSA-N

Formula: C23H36O6

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

Mol. weight [g/mol]: 408.53

Physical Properties

Property code	Value	Unit	Source
gf	-439.07	kJ/mol	Joback Method
hf	-1067.25	kJ/mol	Joback Method
hfus	49.12	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.319		Crippen Method
mcvol	337.790	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2671.00		NIST Webbook
tb	956.47	K	Joback Method
tc	1171.85	K	Joback Method
tf	591.63	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.42	J/mol×K	956.47	Joback Method
cpg	1131.76	J/mol×K	992.37	Joback Method
cpg	1145.55	J/mol×K	1028.26	Joback Method
cpg	1157.83	J/mol×K	1064.16	Joback Method
cpg	1168.60	J/mol×K	1100.06	Joback Method
cpg	1177.90	J/mol×K	1135.95	Joback Method
cpg	1185.73	J/mol×K	1171.85	Joback Method
dvisc	0.0001585	Pa×s	591.63	Joback Method
dvisc	0.0000895	Pa×s	652.44	Joback Method

dvisc	0.0000557	Pa×s	713.24	Joback Method
dvisc	0.0000374	Pa×s	774.05	Joback Method
dvisc	0.0000266	Pa×s	834.86	Joback Method
dvisc	0.0000198	Pa×s	895.66	Joback Method
dvisc	0.0000153	Pa×s	956.47	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369815&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