Diethylmalonic acid, 2,6-dimethoxyphenyl nonyl ester

Inchi: InChI=1S/C24H38O6/c1-6-9-10-11-12-13-14-18-29-22(25)24(7-2,8-3)23(26)30-21-19(27
InchiKey: YAWOELZFWWBZEX-UHFFFAOYSA-N
Formula: C24H38O6
SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 422.55

Physical Properties

Property code	Value	Unit	Source
gf	-430.65	kJ/mol	Joback Method
hf	-1087.89	kJ/mol	Joback Method
hfus	51.71	kJ/mol	Joback Method
hvap	94.45	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.709		Crippen Method
mcvol	351.880	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2765.00		NIST Webbook
tb	979.35	K	Joback Method
tc	1199.05	K	Joback Method
tf	602.90	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.50	J/mol×K	979.35	Joback Method
cpg	1238.52	J/mol×K	1162.43	Joback Method
cpg	1229.50	J/mol×K	1125.81	Joback Method
cpg	1218.91	J/mol×K	1089.20	Joback Method
cpg	1206.73	J/mol×K	1052.58	Joback Method
cpg	1192.94	J/mol×K	1015.97	Joback Method
cpg	1246.01	J/mol×K	1199.05	Joback Method
dvisc	0.0000131	Pa×s	979.35	Joback Method
dvisc	0.0000169	Pa×s	916.61	Joback Method

dvisc	0.0000228	Pa×s	853.87	Joback Method
dvisc	0.0000322	Pa×s	791.12	Joback Method
dvisc	0.0000483	Pa×s	728.38	Joback Method
dvisc	0.0000783	Pa×s	665.64	Joback Method
dvisc	0.0001401	Pa×s	602.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369816&Units=SI

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