Sebacic acid, 2,6-dimethoxyphenyl pentyl ester

Inchi: InChI=1S/C23H36O6/c1-4-5-12-18-28-21(24)16-10-8-6-7-9-11-17-22(25)29-23-19(26-2)1

InchiKey: MRTXDSAAZJSVHQ-UHFFFAOYSA-N

Formula: C23H36O6

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 408.53

Physical Properties

Property code	Value	Unit	Source
gf	-441.91	kJ/mol	Joback Method
hf	-1058.50	kJ/mol	Joback Method
hfus	56.54	kJ/mol	Joback Method
hvap	93.52	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.463		Crippen Method
mcvol	337.790	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	3043.00		NIST Webbook
tb	959.70	K	Joback Method
tc	1174.95	K	Joback Method
tf	589.21	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.25	J/mol×K	959.70	Joback Method
cpg	1131.58	J/mol×K	995.58	Joback Method
cpg	1145.26	J/mol×K	1031.45	Joback Method
cpg	1157.29	J/mol×K	1067.33	Joback Method
cpg	1167.68	J/mol×K	1103.20	Joback Method
cpg	1176.42	J/mol×K	1139.08	Joback Method
cpg	1183.51	J/mol×K	1174.95	Joback Method
dvisc	0.0001843	Pa×s	589.21	Joback Method
dvisc	0.0001068	Pa×s	650.96	Joback Method

dvisc	0.0000681	Pa×s	712.71	Joback Method
dvisc	0.0000466	Pa×s	774.46	Joback Method
dvisc	0.0000337	Pa×s	836.20	Joback Method
dvisc	0.0000255	Pa×s	897.95	Joback Method
dvisc	0.0000200	Pa×s	959.70	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=U354752&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