Isophthalic acid, 2,6-dimethoxyphenyl heptyl ester

Inchi: InChI=1S/C23H28O6/c1-4-5-6-7-8-15-28-22(24)17-11-9-12-18(16-17)23(25)29-21-19(26

InchiKey: HTCKUBUMIUNVMX-UHFFFAOYSA-N

Formula: C23H28O6

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2c(OC)cccc2OC)c1

Mol. weight [g/mol]: 400.46

Physical Properties

Property code	Value	Unit	Source
gf	-339.13	kJ/mol	Joback Method
hf	-833.44	kJ/mol	Joback Method
hfus	50.19	kJ/mol	Joback Method
hvap	96.46	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.050		Crippen Method
mcvol	314.030	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	3164.00		NIST Webbook
tb	991.36	K	Joback Method
tc	1218.17	K	Joback Method
tf	628.15	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.86	J/mol×K	991.36	Joback Method
cpg	1052.39	J/mol×K	1180.36	Joback Method
cpg	1047.12	J/mol×K	1142.56	Joback Method
cpg	1040.14	J/mol×K	1104.76	Joback Method
cpg	1031.43	J/mol×K	1066.96	Joback Method
cpg	1021.01	J/mol×K	1029.16	Joback Method
cpg	1055.93	J/mol×K	1218.17	Joback Method
dvisc	0.0000213	Pa×s	991.36	Joback Method
dvisc	0.0000265	Pa×s	930.83	Joback Method

dvisc	0.0000341	Pa×s	870.29	Joback Method
dvisc	0.0000455	Pa×s	809.76	Joback Method
dvisc	0.0000638	Pa×s	749.22	Joback Method
dvisc	0.0000947	Pa×s	688.69	Joback Method
dvisc	0.0001517	Pa×s	628.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U344537&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