Isophthalic acid, 2,6-dimethoxyphenyl hexyl ester

Inchi: InChI=1S/C22H26O6/c1-4-5-6-7-14-27-21(23)16-10-8-11-17(15-16)22(24)28-20-18(25-2
InchiKey: CRBAGLMZBDUBNK-UHFFFAOYSA-N
Formula: C22H26O6
SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2c(OC)cccc2OC)c1
Mol. weight [g/mol]: 386.44

Physical Properties

Property code	Value	Unit	Source
gf	-347.55	kJ/mol	Joback Method
hf	-812.80	kJ/mol	Joback Method
hfus	47.60	kJ/mol	Joback Method
hvap	94.24	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.660		Crippen Method
mcvol	299.940	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	3062.00		NIST Webbook
tb	968.48	K	Joback Method
tc	1193.61	K	Joback Method
tf	616.88	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.79	J/mol×K	968.48	Joback Method
cpg	962.05	J/mol×K	1006.00	Joback Method
cpg	972.66	J/mol×K	1043.52	Joback Method
cpg	981.63	J/mol×K	1081.04	Joback Method
cpg	988.94	J/mol×K	1118.56	Joback Method
cpg	994.60	J/mol×K	1156.09	Joback Method
cpg	998.61	J/mol×K	1193.61	Joback Method
dvisc	0.0001691	Pa×s	616.88	Joback Method
dvisc	0.0001067	Pa×s	675.48	Joback Method

dvisc	0.0000725	Pa×s	734.08	Joback Method
dvisc	0.0000521	Pa×s	792.68	Joback Method
dvisc	0.0000392	Pa×s	851.28	Joback Method
dvisc	0.0000306	Pa×s	909.88	Joback Method
dvisc	0.0000246	Pa×s	968.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344536&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

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

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