Isophthalic acid, 2,6-dimethoxyphenyl octyl ester

Inchi: InChI=1S/C24H30O6/c1-4-5-6-7-8-9-16-29-23(25)18-12-10-13-19(17-18)24(26)30-22-20

InchiKey: XSFLZJSXZYHCGP-UHFFFAOYSA-N

Formula: C24H30O6

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

Mol. weight [g/mol]: 414.49

Physical Properties

Property code	Value	Unit	Source
gf	-330.71	kJ/mol	Joback Method
hf	-854.08	kJ/mol	Joback Method
hfus	52.78	kJ/mol	Joback Method
hvap	98.69	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.440		Crippen Method
mcvol	328.120	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rinpol	3270.00		NIST Webbook
tb	1014.24	K	Joback Method
tc	1243.67	K	Joback Method
tf	639.42	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.32	J/mol×K	1014.24	Joback Method
cpg	1080.33	J/mol×K	1052.48	Joback Method
cpg	1090.54	J/mol×K	1090.72	Joback Method
cpg	1098.94	J/mol×K	1128.95	Joback Method
cpg	1105.53	J/mol×K	1167.19	Joback Method
cpg	1110.33	J/mol×K	1205.43	Joback Method
cpg	1113.34	J/mol×K	1243.67	Joback Method
dvisc	0.0001357	Pa×s	639.42	Joback Method
dvisc	0.0000838	Pa×s	701.89	Joback Method

dvisc	0.0000560	Pa×s	764.36	Joback Method
dvisc	0.0000397	Pa×s	826.83	Joback Method
dvisc	0.0000296	Pa×s	889.30	Joback Method
dvisc	0.0000229	Pa×s	951.77	Joback Method
dvisc	0.0000183	Pa×s	1014.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344538&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