Terephthalic acid, di(3-methoxyphenyl) ester

Inchi: InChI=1S/C22H18O6/c1-25-17-5-3-7-19(13-17)27-21(23)15-9-11-16(12-10-15)22(24)28-
InchiKey: KODPEPBVDZOCQM-UHFFFAOYSA-N
Formula: C22H18O6
SMILES: COc1cccc(OC(=O)c2ccc(C(=O)Oc3cccc(OC)c3)cc2)c1
Mol. weight [g/mol]: 378.37

Physical Properties

Property code	Value	Unit	Source
gf	-235.14	kJ/mol	Joback Method
hf	-576.27	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	96.51	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.142		Crippen Method
mcvol	276.180	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	995.16	K	Joback Method
tc	1242.86	K	Joback Method
tf	643.30	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.46	J/mol×K	995.16	Joback Method
cpg	849.96	J/mol×K	1036.44	Joback Method
cpg	857.62	J/mol×K	1077.73	Joback Method
cpg	863.47	J/mol×K	1119.01	Joback Method
cpg	867.49	J/mol×K	1160.29	Joback Method
cpg	869.70	J/mol×K	1201.58	Joback Method
cpg	870.11	J/mol×K	1242.86	Joback Method
dvisc	0.0001575	Pa×s	643.30	Joback Method

dvisc	0.0001025	Pa×s	701.94	Joback Method
dvisc	0.0000713	Pa×s	760.59	Joback Method
dvisc	0.0000522	Pa×s	819.23	Joback Method
dvisc	0.0000398	Pa×s	877.87	Joback Method
dvisc	0.0000315	Pa×s	936.52	Joback Method
dvisc	0.0000256	Pa×s	995.16	Joback Method

Sources

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=U415826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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