Isophthalic acid, di(3-methylphenyl) ester

Inchi: InChI=1S/C22H18O4/c1-15-6-3-10-19(12-15)25-21(23)17-8-5-9-18(14-17)22(24)26-20-1
InchiKey: PTZZYDVLRWPZNJ-UHFFFAOYSA-N
Formula: C22H18O4
SMILES: Cc1cccc(OC(=O)c2cccc(C(=O)Oc3cccc(C)c3)c2)c1
Mol. weight [g/mol]: 346.38

Physical Properties

Property code	Value	Unit	Source
gf	-25.14	kJ/mol	Joback Method
hf	-311.83	kJ/mol	Joback Method
hfus	39.27	kJ/mol	Joback Method
hvap	91.69	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	4.742		Crippen Method
mcvol	264.440	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	3079.00		NIST Webbook
rinpol	3079.00		NIST Webbook
tb	950.32	K	Joback Method
tc	1201.35	K	Joback Method
tf	598.84	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.76	J/mol×K	950.32	Joback Method
cpg	802.62	J/mol×K	992.16	Joback Method
cpg	812.95	J/mol×K	1034.00	Joback Method
cpg	821.82	J/mol×K	1075.83	Joback Method
cpg	829.28	J/mol×K	1117.67	Joback Method
cpg	835.38	J/mol×K	1159.51	Joback Method
cpg	840.17	J/mol×K	1201.35	Joback Method
dvisc	0.0003041	Pa×s	598.84	Joback Method

dvisc	0.0001927	Pa×s	657.42	Joback Method
dvisc	0.0001316	Pa×s	716.00	Joback Method
dvisc	0.0000952	Pa×s	774.58	Joback Method
dvisc	0.0000721	Pa×s	833.16	Joback Method
dvisc	0.0000566	Pa×s	891.74	Joback Method
dvisc	0.0000458	Pa×s	950.32	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=U344523&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