Isophthalic acid, di(3,4-dimethylphenyl) ester

Inchi: InChI=1S/C24H22O4/c1-15-8-10-21(12-17(15)3)27-23(25)19-6-5-7-20(14-19)24(26)28-2
InchiKey: DKURDVKTTOEVAP-UHFFFAOYSA-N
Formula: C24H22O4
SMILES: Cc1ccc(OC(=O)c2cccc(C(=O)Oc3ccc(C)c(C)c3)c2)cc1C
Mol. weight [g/mol]: 374.43

Physical Properties

Property code	Value	Unit	Source
gf	-27.56	kJ/mol	Joback Method
hf	-376.05	kJ/mol	Joback Method
hfus	43.67	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	5.359		Crippen Method
mcvol	292.620	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	3289.00		NIST Webbook
rinpol	3289.00		NIST Webbook
tb	1006.04	K	Joback Method
tc	1253.82	K	Joback Method
tf	646.42	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.58	J/mol×K	1006.04	Joback Method
cpg	944.98	J/mol×K	1212.52	Joback Method
cpg	939.74	J/mol×K	1171.22	Joback Method
cpg	933.02	J/mol×K	1129.93	Joback Method
cpg	924.78	J/mol×K	1088.63	Joback Method
cpg	914.98	J/mol×K	1047.34	Joback Method
cpg	948.77	J/mol×K	1253.82	Joback Method
dvisc	0.0000366	Pa×s	1006.04	Joback Method

dvisc	0.0000446	Pa×s	946.10	Joback Method
dvisc	0.0000558	Pa×s	886.17	Joback Method
dvisc	0.0000723	Pa×s	826.23	Joback Method
dvisc	0.0000974	Pa×s	766.29	Joback Method
dvisc	0.0001380	Pa×s	706.36	Joback Method
dvisc	0.0002088	Pa×s	646.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344450&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