Isophthalic acid, di(2-ethylphenyl) ester

Inchi: InChI=1S/C24H22O4/c1-3-17-10-5-7-14-21(17)27-23(25)19-12-9-13-20(16-19)24(26)28-
InchiKey: BCMNPNDTIQWFJZ-UHFFFAOYSA-N
Formula: C24H22O4
SMILES: CCc1ccccc1OC(=O)c1cccc(C(=O)Oc2ccccc2CC)c1
Mol. weight [g/mol]: 374.43

Physical Properties

Property code	Value	Unit	Source
gf	-8.30	kJ/mol	Joback Method
hf	-353.11	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	96.14	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.250		Crippen Method
mcvol	292.620	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	3001.00		NIST Webbook
rinpol	3001.00		NIST Webbook
tb	996.08	K	Joback Method
tc	1242.38	K	Joback Method
tf	621.38	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.66	J/mol×K	996.08	Joback Method
cpg	950.85	J/mol×K	1201.33	Joback Method
cpg	944.82	J/mol×K	1160.28	Joback Method
cpg	937.44	J/mol×K	1119.23	Joback Method
cpg	928.67	J/mol×K	1078.18	Joback Method
cpg	918.43	J/mol×K	1037.13	Joback Method
cpg	955.60	J/mol×K	1242.38	Joback Method
dvisc	0.0000346	Pa×s	996.08	Joback Method

dvisc	0.0000431	Pa×s	933.63	Joback Method
dvisc	0.0000553	Pa×s	871.18	Joback Method
dvisc	0.0000738	Pa×s	808.73	Joback Method
dvisc	0.0001034	Pa×s	746.28	Joback Method
dvisc	0.0001539	Pa×s	683.83	Joback Method
dvisc	0.0002483	Pa×s	621.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356767&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