Isophthalic acid, pentyl phenyl ester

Inchi: InChI=1S/C19H20O4/c1-2-3-7-13-22-18(20)15-9-8-10-16(14-15)19(21)23-17-11-5-4-6-12
InchiKey: YNVFDIIIEYACTD-UHFFFAOYSA-N
Formula: C19H20O4
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]: 312.36

Physical Properties

Property code	Value	Unit	Source
gf	-143.55	kJ/mol	Joback Method
hf	-463.50	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	81.41	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.253		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2581.00		NIST Webbook
tb	845.04	K	Joback Method
tc	1070.91	K	Joback Method
tf	513.57	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.43	J/mol×K	845.04	Joback Method
cpg	782.63	J/mol×K	1033.27	Joback Method
cpg	773.37	J/mol×K	995.62	Joback Method
cpg	762.96	J/mol×K	957.98	Joback Method
cpg	751.35	J/mol×K	920.33	Joback Method
cpg	738.52	J/mol×K	882.69	Joback Method
cpg	790.77	J/mol×K	1070.91	Joback Method
dvisc	0.0000643	Pa×s	845.04	Joback Method
dvisc	0.0000814	Pa×s	789.79	Joback Method

dvisc	0.0001068	Pa×s	734.55	Joback Method
dvisc	0.0001464	Pa×s	679.30	Joback Method
dvisc	0.0002123	Pa×s	624.06	Joback Method
dvisc	0.0003309	Pa×s	568.81	Joback Method
dvisc	0.0005675	Pa×s	513.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344358&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