Isophthalic acid, pentachlorophenyl propyl ester

Inchi: InChI=1S/C17H11Cl5O4/c1-2-6-25-16(23)8-4-3-5-9(7-8)17(24)26-15-13(21)11(19)10(18)
InchiKey: OAQGQSMDENMZRR-UHFFFAOYSA-N
Formula: C17H11Cl5O4
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]: 456.53

Physical Properties

Property code	Value	Unit	Source
gf	-268.19	kJ/mol	Joback Method
hf	-558.27	kJ/mol	Joback Method
hfus	52.09	kJ/mol	Joback Method
hvap	102.20	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	6.740		Crippen Method
mcvol	278.950	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	3120.00		NIST Webbook
tb	1011.33	K	Joback Method
tc	1260.86	K	Joback Method
tf	703.23	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.44	J/mol×K	1011.33	Joback Method
cpg	705.86	J/mol×K	1052.92	Joback Method
cpg	710.98	J/mol×K	1094.51	Joback Method
cpg	714.82	J/mol×K	1136.10	Joback Method
cpg	717.39	J/mol×K	1177.69	Joback Method
cpg	718.68	J/mol×K	1219.28	Joback Method
cpg	718.70	J/mol×K	1260.86	Joback Method
dvisc	0.0001826	Pa×s	703.23	Joback Method
dvisc	0.0001331	Pa×s	754.58	Joback Method

dvisc	0.0001011	Pa×s	805.93	Joback Method
dvisc	0.0000793	Pa×s	857.28	Joback Method
dvisc	0.0000639	Pa×s	908.63	Joback Method
dvisc	0.0000528	Pa×s	959.98	Joback Method
dvisc	0.0000444	Pa×s	1011.33	Joback Method

Sources

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=U356574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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