Isophthalic acid, 2,6-dichlorophenyl hexyl ester

Inchi: InChI=1S/C20H20Cl2O4/c1-2-3-4-5-12-25-19(23)14-8-6-9-15(13-14)20(24)26-18-16(21)1

InchiKey: QENVYIGPEXGPOK-UHFFFAOYSA-N

Formula: C20H20Cl2O4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cccc2Cl)c1

Mol. weight [g/mol]: 395.28

Physical Properties

Property code	Value	Unit	Source
gf	-178.25	kJ/mol	Joback Method
hf	-538.56	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.950		Crippen Method
mcvol	284.500	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2955.00		NIST Webbook
tb	952.74	K	Joback Method
tc	1185.41	K	Joback Method
tf	609.72	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.06	J/mol×K	952.74	Joback Method
cpg	834.27	J/mol×K	991.52	Joback Method
cpg	844.20	J/mol×K	1030.30	Joback Method
cpg	852.87	J/mol×K	1069.08	Joback Method
cpg	860.32	J/mol×K	1107.86	Joback Method
cpg	866.57	J/mol×K	1146.64	Joback Method
cpg	871.66	J/mol×K	1185.41	Joback Method
dvisc	0.0002844	Pa×s	609.72	Joback Method

dvisc	0.0001817	Pa×s	666.89	Joback Method
dvisc	0.0001246	Pa×s	724.06	Joback Method
dvisc	0.0000903	Pa×s	781.23	Joback Method
dvisc	0.0000684	Pa×s	838.40	Joback Method
dvisc	0.0000537	Pa×s	895.57	Joback Method
dvisc	0.0000433	Pa×s	952.74	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=U344624&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