Isophthalic acid, 3,5-dichlorophenyl isohexyl ester

Inchi: InChI=1S/C20H20Cl2O4/c1-13(2)5-4-8-25-19(23)14-6-3-7-15(9-14)20(24)26-18-11-16(21

InchiKey: YWKANXXECNCBKO-UHFFFAOYSA-N

Formula: C20H20Cl2O4

SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2)c1

Mol. weight [g/mol]: 395.28

Physical Properties

Property code	Value	Unit	Source
gf	-180.69	kJ/mol	Joback Method
hf	-543.84	kJ/mol	Joback Method
hfus	44.92	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.806		Crippen Method
mcvol	284.500	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2874.00		NIST Webbook
tb	952.30	K	Joback Method
tc	1187.41	K	Joback Method
tf	594.72	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.54	J/mol×K	952.30	Joback Method
cpg	866.94	J/mol×K	1148.23	Joback Method
cpg	860.79	J/mol×K	1109.04	Joback Method
cpg	853.41	J/mol×K	1069.86	Joback Method
cpg	844.76	J/mol×K	1030.67	Joback Method
cpg	834.82	J/mol×K	991.49	Joback Method
cpg	871.89	J/mol×K	1187.41	Joback Method
dvisc	0.0000395	Pa×s	952.30	Joback Method
dvisc	0.0000495	Pa×s	892.70	Joback Method

dvisc	0.0000641	Pa×s	833.11	Joback Method
dvisc	0.0000864	Pa×s	773.51	Joback Method
dvisc	0.0001223	Pa×s	713.91	Joback Method
dvisc	0.0001846	Pa×s	654.32	Joback Method
dvisc	0.0003024	Pa×s	594.72	Joback Method

Sources

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=U356584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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