Isophthalic acid, di(2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C22H28Cl2O4/c23-19-10-3-1-6-17(19)13-27-21(25)15-8-5-9-16(12-15)22(26)2
InchiKey: PZGVJALZLRDDFL-UHFFFAOYSA-N
Formula: C22H28Cl2O4
SMILES: O=C(OCC1CCCCC1Cl)c1cccc(C(=O)OCC2CCCCC2Cl)c1
Mol. weight [g/mol]: 427.36

Physical Properties

Property code	Value	Unit	Source
gf	-221.08	kJ/mol	Joback Method
hf	-725.47	kJ/mol	Joback Method
hfus	46.17	kJ/mol	Joback Method
hvap	94.83	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.595		Crippen Method
mcvol	314.720	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	3454.00		NIST Webbook
rinpol	3454.00		NIST Webbook
tb	991.62	K	Joback Method
tc	1237.27	K	Joback Method
tf	587.08	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.82	J/mol×K	991.62	Joback Method
cpg	1058.56	J/mol×K	1032.56	Joback Method
cpg	1070.12	J/mol×K	1073.50	Joback Method
cpg	1079.56	J/mol×K	1114.45	Joback Method
cpg	1086.92	J/mol×K	1155.39	Joback Method
cpg	1092.24	J/mol×K	1196.33	Joback Method
cpg	1095.57	J/mol×K	1237.27	Joback Method
dvisc	0.0005200	Pa×s	587.08	Joback Method

dvisc	0.0002968	Pa×s	654.50	Joback Method
dvisc	0.0001881	Pa×s	721.93	Joback Method
dvisc	0.0001289	Pa×s	789.35	Joback Method
dvisc	0.0000937	Pa×s	856.77	Joback Method
dvisc	0.0000714	Pa×s	924.20	Joback Method
dvisc	0.0000564	Pa×s	991.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343799&Units=SI

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