Isophthalic acid, (2-chlorocyclohexyl)methyl heptyl ester

Inchi: InChI=1S/C22H31ClO4/c1-2-3-4-5-8-14-26-21(24)17-11-9-12-18(15-17)22(25)27-16-19-1

InchiKey: IHEFHSFJEJWNKH-UHFFFAOYSA-N

Formula: C22H31ClO4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2Cl)c1

Mol. weight [g/mol]: 394.93

Physical Properties

Property code	Value	Unit	Source
gf	-225.89	kJ/mol	Joback Method
hf	-743.71	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	90.32	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	5.768		Crippen Method
mcvol	313.340	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	3087.00		NIST Webbook
rinpol	3087.00		NIST Webbook
tb	939.31	K	Joback Method
tc	1161.55	K	Joback Method
tf	554.02	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.20	J/mol×K	939.31	Joback Method
cpg	1085.03	J/mol×K	1124.51	Joback Method
cpg	1075.76	J/mol×K	1087.47	Joback Method
cpg	1064.98	J/mol×K	1050.43	Joback Method
cpg	1052.65	J/mol×K	1013.39	Joback Method
cpg	1038.74	J/mol×K	976.35	Joback Method
cpg	1092.82	J/mol×K	1161.55	Joback Method
dvisc	0.0000481	Pa×s	939.31	Joback Method

dvisc	0.0000615	Pa×s	875.09	Joback Method
dvisc	0.0000817	Pa×s	810.88	Joback Method
dvisc	0.0001141	Pa×s	746.66	Joback Method
dvisc	0.0001697	Pa×s	682.45	Joback Method
dvisc	0.0002740	Pa×s	618.24	Joback Method
dvisc	0.0004944	Pa×s	554.02	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=U343798&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