Isophthalic acid, (2-chlorocyclohexyl)methyl isohexyl ester

Inchi: InChI=1S/C21H29ClO4/c1-15(2)7-6-12-25-20(23)16-9-5-10-17(13-16)21(24)26-14-18-8-3

InchiKey: ANCPDJAIGGZLQF-UHFFFAOYSA-N

Formula: C21H29ClO4

SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)OCC2CCCCC2Cl)c1

Mol. weight [g/mol]: 380.91

Physical Properties

Property code	Value	Unit	Source
gf	-236.75	kJ/mol	Joback Method
hf	-728.35	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	87.71	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.234		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2927.00		NIST Webbook
rinpol	2927.00		NIST Webbook
tb	915.99	K	Joback Method
tc	1140.34	K	Joback Method
tf	527.75	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.64	J/mol×K	915.99	Joback Method
cpg	1026.44	J/mol×K	1102.95	Joback Method
cpg	1017.01	J/mol×K	1065.56	Joback Method
cpg	1006.05	J/mol×K	1028.17	Joback Method
cpg	993.52	J/mol×K	990.77	Joback Method
cpg	979.39	J/mol×K	953.38	Joback Method
cpg	1034.38	J/mol×K	1140.34	Joback Method
dvisc	0.0000506	Pa×s	915.99	Joback Method

dvisc	0.0000655	Pa×s	851.28	Joback Method
dvisc	0.0000883	Pa×s	786.58	Joback Method
dvisc	0.0001256	Pa×s	721.87	Joback Method
dvisc	0.0001914	Pa×s	657.16	Joback Method
dvisc	0.0003200	Pa×s	592.46	Joback Method
dvisc	0.0006069	Pa×s	527.75	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=U343796&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