

Isophthalic acid, 2-chlorophenyl octyl ester

Inchi:	InChI=1S/C22H25ClO4/c1-2-3-4-5-6-9-15-26-21(24)17-11-10-12-18(16-17)22(25)27-20-
InchiKey:	VWQVNPPUFSVEMI-UHFFFAOYSA-N
Formula:	C22H25ClO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2Cl)c1
Mol. weight [g/mol]:	388.88

Physical Properties

Property code	Value	Unit	Source
gf	-139.85	kJ/mol	Joback Method
hf	-552.63	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	93.14	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.077		Crippen Method
mvol	300.440	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	3057.00		NIST Webbook
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tb	956.09	K	Joback Method
tc	1183.10	K	Joback Method
tf	589.82	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.72	J/molxK	956.09	Joback Method
cpg	932.57	J/molxK	993.93	Joback Method
cpg	944.09	J/molxK	1031.76	Joback Method
cpg	954.31	J/molxK	1069.60	Joback Method
cpg	963.29	J/molxK	1107.43	Joback Method
cpg	971.07	J/molxK	1145.27	Joback Method
cpg	977.69	J/molxK	1183.10	Joback Method
dvisc	0.0003074	Paxs	589.82	Joback Method

dvisc	0.0001832	Paxs	650.87	Joback Method
dvisc	0.0001193	Paxs	711.91	Joback Method
dvisc	0.0000832	Paxs	772.95	Joback Method
dvisc	0.0000611	Paxs	834.00	Joback Method
dvisc	0.0000468	Paxs	895.04	Joback Method
dvisc	0.0000371	Paxs	956.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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