

Isophthalic acid, monochloride, phenyl ester

Inchi:	InChI=1S/C14H9ClO3/c15-13(16)10-5-4-6-11(9-10)14(17)18-12-7-2-1-3-8-12/h1-9H
InchiKey:	RPVOSOKUGZNNQU-UHFFFAOYSA-N
Formula:	C14H9ClO3
SMILES:	O=C(Cl)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]:	260.67

Physical Properties

Property code	Value	Unit	Source
gf	-92.58	kJ/mol	Joback Method
hf	-243.82	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	72.26	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.285		Crippen Method
mvol	181.850	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	2328.00		NIST Webbook
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tb	745.65	K	Joback Method
tc	996.99	K	Joback Method
tf	464.91	K	Joback Method
vc	0.682	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.76	J/molxK	745.65	Joback Method
cpg	499.22	J/molxK	955.10	Joback Method
cpg	491.62	J/molxK	913.21	Joback Method
cpg	483.02	J/molxK	871.32	Joback Method
cpg	473.38	J/molxK	829.43	Joback Method
cpg	462.65	J/molxK	787.54	Joback Method
cpg	505.88	J/molxK	996.99	Joback Method
dvisc	0.0001417	Paxs	745.65	Joback Method

dvisc	0.0001763	Paxs	698.86	Joback Method
dvisc	0.0002262	Paxs	652.07	Joback Method
dvisc	0.0003017	Paxs	605.28	Joback Method
dvisc	0.0004224	Paxs	558.49	Joback Method
dvisc	0.0006288	Paxs	511.70	Joback Method
dvisc	0.0010141	Paxs	464.91	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344366&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

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