

Isophthalic acid, di(2-chloroethyl) ester

Inchi:	InChI=1S/C12H12Cl2O4/c13-4-6-17-11(15)9-2-1-3-10(8-9)12(16)18-7-5-14/h1-3,8H,4-7H
InchiKey:	UZZVLAWGGKYCLD-UHFFFAOYSA-N
Formula:	C12H12Cl2O4
SMILES:	O=C(OCCCl)c1cccc(C(=O)OCCCl)c1
Mol. weight [g/mol]:	291.13

Physical Properties

Property code	Value	Unit	Source
gf	-338.76	kJ/mol	Joback Method
hf	-587.03	kJ/mol	Joback Method
hfus	34.46	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.478		Crippen Method
mvol	195.540	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	733.06	K	Joback Method
tc	951.25	K	Joback Method
tf	468.10	K	Joback Method
vc	0.746	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.74	J/molxK	733.06	Joback Method
cpg	496.09	J/molxK	769.43	Joback Method
cpg	506.58	J/molxK	805.79	Joback Method
cpg	516.22	J/molxK	842.16	Joback Method
cpg	525.03	J/molxK	878.52	Joback Method
cpg	533.00	J/molxK	914.89	Joback Method
cpg	540.14	J/molxK	951.25	Joback Method
dvisc	0.0008555	Paxs	468.10	Joback Method

dvisc	0.0005397	Paxs	512.26	Joback Method
dvisc	0.0003663	Paxs	556.42	Joback Method
dvisc	0.0002632	Paxs	600.58	Joback Method
dvisc	0.0001978	Paxs	644.74	Joback Method
dvisc	0.0001543	Paxs	688.90	Joback Method
dvisc	0.0001240	Paxs	733.06	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=U345875&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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