

Isophthalic acid, 2,5-dichlorophenyl ethyl ester

Inchi:	InChI=1S/C16H12Cl2O4/c1-2-21-15(19)10-4-3-5-11(8-10)16(20)22-14-9-12(17)6-7-13(14)
InchiKey:	GJRJFCUEDNCZHQ-UHFFFAOYSA-N
Formula:	C16H12Cl2O4
SMILES:	CCOC(=O)c1cccc(C(=O)Oc2cc(Cl)ccc2Cl)c1
Mol. weight [g/mol]:	339.17

Physical Properties

Property code	Value	Unit	Source
gf	-211.93	kJ/mol	Joback Method
hf	-456.00	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	84.83	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.389		Crippen Method
mvol	228.140	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	2587.00		NIST Webbook
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tb	861.22	K	Joback Method
tc	1103.13	K	Joback Method
tf	564.64	K	Joback Method
vc	0.862	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.64	J/molxK	861.22	Joback Method
cpg	609.25	J/molxK	901.54	Joback Method
cpg	618.67	J/molxK	941.86	Joback Method
cpg	626.91	J/molxK	982.17	Joback Method
cpg	634.01	J/molxK	1022.49	Joback Method
cpg	639.97	J/molxK	1062.81	Joback Method
cpg	644.82	J/molxK	1103.13	Joback Method
dvisc	0.0004213	Paxs	564.64	Joback Method

dvisc	0.0002823	Paxs	614.07	Joback Method
dvisc	0.0002007	Paxs	663.50	Joback Method
dvisc	0.0001497	Paxs	712.93	Joback Method
dvisc	0.0001159	Paxs	762.36	Joback Method
dvisc	0.0000926	Paxs	811.79	Joback Method
dvisc	0.0000759	Paxs	861.22	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=U344696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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