

Isophthalic acid, ethyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C16H11Cl3O4/c1-2-22-15(20)9-4-3-5-10(6-9)16(21)23-14-12(18)7-11(17)8-13
InchiKey:	FZSRBJKOTUCYHG-UHFFFAOYSA-N
Formula:	C16H11Cl3O4
SMILES:	CCOC(=O)c1cccc(C(=O)Oc2c(Cl)cc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	373.62

Physical Properties

Property code	Value	Unit	Source
gf	-233.49	kJ/mol	Joback Method
hf	-483.21	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.043		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2677.00		NIST Webbook
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tb	903.63	K	Joback Method
tc	1148.58	K	Joback Method
tf	607.08	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.69	J/molxK	903.63	Joback Method
cpg	649.73	J/molxK	1107.75	Joback Method
cpg	645.26	J/molxK	1066.93	Joback Method
cpg	639.63	J/molxK	1026.10	Joback Method
cpg	632.83	J/molxK	985.28	Joback Method
cpg	624.86	J/molxK	944.45	Joback Method
cpg	653.06	J/molxK	1148.58	Joback Method
dvisc	0.0000671	Paxs	903.63	Joback Method

dvisc	0.0000810	Paxs	854.20	Joback Method
dvisc	0.0000999	Paxs	804.78	Joback Method
dvisc	0.0001268	Paxs	755.36	Joback Method
dvisc	0.0001664	Paxs	705.93	Joback Method
dvisc	0.0002274	Paxs	656.50	Joback Method
dvisc	0.0003270	Paxs	607.08	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=U344565&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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