

Isophthalic acid, propyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C17H13Cl3O4/c1-2-6-23-16(21)10-4-3-5-11(7-10)17(22)24-14-9-12(18)8-13(19)
InchiKey:	MZJAONDRHYRYLM-UHFFFAOYSA-N
Formula:	C17H13Cl3O4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2Cl)c1
Mol. weight [g/mol]:	387.64

Physical Properties

Property code	Value	Unit	Source
gf	-225.07	kJ/mol	Joback Method
hf	-503.85	kJ/mol	Joback Method
hfus	44.48	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.433		Crippen Method
mcvol	254.470	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2761.00		NIST Webbook
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tb	926.51	K	Joback Method
tc	1168.45	K	Joback Method
tf	618.35	K	Joback Method
vc	0.967	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.85	J/molxK	926.51	Joback Method
cpg	705.65	J/molxK	1128.13	Joback Method
cpg	701.07	J/molxK	1087.81	Joback Method
cpg	695.31	J/molxK	1047.48	Joback Method
cpg	688.37	J/molxK	1007.16	Joback Method
cpg	680.22	J/molxK	966.83	Joback Method
cpg	709.08	J/molxK	1168.45	Joback Method
dvisc	0.0000583	Paxs	926.51	Joback Method

dvisc	0.0000706	Paxs	875.15	Joback Method
dvisc	0.0000876	Paxs	823.79	Joback Method
dvisc	0.0001118	Paxs	772.43	Joback Method
dvisc	0.0001478	Paxs	721.07	Joback Method
dvisc	0.0002038	Paxs	669.71	Joback Method
dvisc	0.0002965	Paxs	618.35	Joback Method

Sources

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=U356617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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