

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

Inchi:	InChI=1S/C18H15Cl3O4/c1-10(2)9-24-17(22)11-4-3-5-12(6-11)18(23)25-16-14(20)7-13(
InchiKey:	MWYBZEYXTKZBEQ-UHFFFAOYSA-N
Formula:	C18H15Cl3O4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)Oc2c(Cl)cc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	401.67

Physical Properties

Property code	Value	Unit	Source
gf	-219.09	kJ/mol	Joback Method
hf	-529.77	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.679		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2821.00		NIST Webbook
rinpol	2821.00		NIST Webbook
tb	948.95	K	Joback Method
tc	1191.57	K	Joback Method
tf	614.62	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.27	J/molxK	948.95	Joback Method
cpg	736.84	J/molxK	989.39	Joback Method
cpg	745.12	J/molxK	1029.82	Joback Method
cpg	752.13	J/molxK	1070.26	Joback Method
cpg	757.88	J/molxK	1110.70	Joback Method
cpg	762.39	J/molxK	1151.13	Joback Method
cpg	765.69	J/molxK	1191.57	Joback Method
dvisc	0.0002812	Paxs	614.62	Joback Method

dvisc	0.0001835	Paxs	670.34	Joback Method
dvisc	0.0001279	Paxs	726.06	Joback Method
dvisc	0.0000938	Paxs	781.79	Joback Method
dvisc	0.0000717	Paxs	837.51	Joback Method
dvisc	0.0000567	Paxs	893.23	Joback Method
dvisc	0.0000461	Paxs	948.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344567&Units=SI
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

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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