

Isophthalic acid, 2,6-dichlorophenyl isobutyl ester

Inchi:	InChI=1S/C18H16Cl2O4/c1-11(2)10-23-17(21)12-5-3-6-13(9-12)18(22)24-16-14(19)7-4-8
InchiKey:	NOIFNHPGLOUFLM-UHFFFAOYSA-N
Formula:	C18H16Cl2O4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)Oc2c(Cl)cccc2Cl)c1
Mol. weight [g/mol]:	367.22

Physical Properties

Property code	Value	Unit	Source
gf	-197.53	kJ/mol	Joback Method
hf	-502.56	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.025		Crippen Method
mvol	256.320	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2692.00		NIST Webbook
rinpol	2692.00		NIST Webbook
tb	906.54	K	Joback Method
tc	1145.54	K	Joback Method
tf	572.18	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.90	J/molxK	906.54	Joback Method
cpg	752.79	J/molxK	1105.71	Joback Method
cpg	746.68	J/molxK	1065.87	Joback Method
cpg	739.36	J/molxK	1026.04	Joback Method
cpg	730.81	J/molxK	986.21	Joback Method
cpg	721.00	J/molxK	946.37	Joback Method
cpg	757.72	J/molxK	1145.54	Joback Method
dvisc	0.0000527	Paxs	906.54	Joback Method

dvisc	0.0000656	Paxs	850.81	Joback Method
dvisc	0.0000842	Paxs	795.09	Joback Method
dvisc	0.0001123	Paxs	739.36	Joback Method
dvisc	0.0001569	Paxs	683.63	Joback Method
dvisc	0.0002327	Paxs	627.91	Joback Method
dvisc	0.0003726	Paxs	572.18	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=U344620&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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