

Isophthalic acid, 3-chlorophenyl isobutyl ester

Inchi:	InChI=1S/C18H17ClO4/c1-12(2)11-22-17(20)13-5-3-6-14(9-13)18(21)23-16-8-4-7-15(19)
InchiKey:	OYNGDJFIDBKFQD-UHFFFAOYSA-N
Formula:	C18H17ClO4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]:	332.78

Physical Properties

Property code	Value	Unit	Source
gf	-175.97	kJ/mol	Joback Method
hf	-475.35	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	83.85	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.372		Crippen Method
mcvol	244.080	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2605.00		NIST Webbook
tb	864.13	K	Joback Method
tc	1099.69	K	Joback Method
tf	529.74	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.43	J/molxK	864.13	Joback Method
cpg	703.05	J/molxK	903.39	Joback Method
cpg	714.38	J/molxK	942.65	Joback Method
cpg	724.45	J/molxK	981.91	Joback Method
cpg	733.30	J/molxK	1021.17	Joback Method
cpg	740.96	J/molxK	1060.43	Joback Method
cpg	747.45	J/molxK	1099.69	Joback Method
dvisc	0.0005029	Paxs	529.74	Joback Method
dvisc	0.0002978	Paxs	585.47	Joback Method

dvisc	0.0001932	Paxs	641.20	Joback Method
dvisc	0.0001343	Paxs	696.93	Joback Method
dvisc	0.0000985	Paxs	752.67	Joback Method
dvisc	0.0000754	Paxs	808.40	Joback Method
dvisc	0.0000598	Paxs	864.13	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=U344601&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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