

Isophthalic acid, butyl 4-chlorophenyl ester

Inchi:	InChI=1S/C18H17ClO4/c1-2-3-11-22-17(20)13-5-4-6-14(12-13)18(21)23-16-9-7-15(19)8
InchiKey:	AYKQEOHABKNHQA-UHFFFAOYSA-N
Formula:	C18H17ClO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]:	332.78

Physical Properties

Property code	Value	Unit	Source
gf	-173.53	kJ/mol	Joback Method
hf	-470.07	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.516		Crippen Method
mcvol	244.080	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2680.00		NIST Webbook
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tb	864.57	K	Joback Method
tc	1096.73	K	Joback Method
tf	544.74	K	Joback Method
vc	0.924	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.86	J/molxK	864.57	Joback Method
cpg	702.33	J/molxK	903.26	Joback Method
cpg	713.55	J/molxK	941.96	Joback Method
cpg	723.58	J/molxK	980.65	Joback Method
cpg	732.42	J/molxK	1019.35	Joback Method
cpg	740.12	J/molxK	1058.04	Joback Method
cpg	746.70	J/molxK	1096.73	Joback Method
dvisc	0.0004610	Paxs	544.74	Joback Method

dvisc	0.0002879	Paxs	598.04	Joback Method
dvisc	0.0001942	Paxs	651.35	Joback Method
dvisc	0.0001390	Paxs	704.65	Joback Method
dvisc	0.0001043	Paxs	757.96	Joback Method
dvisc	0.0000813	Paxs	811.26	Joback Method
dvisc	0.0000653	Paxs	864.57	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=U344578&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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