

Isophthalic acid, butyl 2,4-dichlorophenyl ester

Inchi:	InChI=1S/C18H16Cl2O4/c1-2-3-9-23-17(21)12-5-4-6-13(10-12)18(22)24-16-8-7-14(19)1
InchiKey:	MCVACCBINRBMMT-UHFFFAOYSA-N
Formula:	C18H16Cl2O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	367.22

Physical Properties

Property code	Value	Unit	Source
gf	-195.09	kJ/mol	Joback Method
hf	-497.28	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.170		Crippen Method
mcvol	256.320	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	906.98	K	Joback Method
tc	1142.81	K	Joback Method
tf	587.18	K	Joback Method
vc	0.974	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.35	J/molxK	906.98	Joback Method
cpg	720.35	J/molxK	946.28	Joback Method
cpg	730.10	J/molxK	985.59	Joback Method
cpg	738.64	J/molxK	1024.89	Joback Method
cpg	746.00	J/molxK	1064.20	Joback Method
cpg	752.20	J/molxK	1103.50	Joback Method
cpg	757.26	J/molxK	1142.81	Joback Method
dvisc	0.0003488	Paxs	587.18	Joback Method

dvisc	0.0002281	Paxs	640.48	Joback Method
dvisc	0.0001592	Paxs	693.78	Joback Method
dvisc	0.0001170	Paxs	747.08	Joback Method
dvisc	0.0000895	Paxs	800.38	Joback Method
dvisc	0.0000709	Paxs	853.68	Joback Method
dvisc	0.0000577	Paxs	906.98	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=U344407&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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