

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

Other names:	2,4,6-Trichlorophenol, isoBOC
Inchi:	InChI=1S/C11H11Cl3O3/c1-6(2)5-16-11(15)17-10-8(13)3-7(12)4-9(10)14/h3-4,6H,5H2,1
InchiKey:	UDQGNCNQSIVYSON-UHFFFAOYSA-N
Formula:	C11H11Cl3O3
SMILES:	CC(C)COC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	297.56

Physical Properties

Property code	Value	Unit	Source
gf	-251.89	kJ/mol	Joback Method
hf	-497.77	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.818		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1771.00		NIST Webbook
tb	703.26	K	Joback Method
tc	927.66	K	Joback Method
tf	446.86	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.25	J/molxK	703.26	Joback Method
cpg	491.50	J/molxK	890.26	Joback Method
cpg	483.43	J/molxK	852.86	Joback Method
cpg	474.56	J/molxK	815.46	Joback Method
cpg	464.90	J/molxK	778.06	Joback Method
cpg	454.46	J/molxK	740.66	Joback Method
cpg	498.78	J/molxK	927.66	Joback Method
dvisc	0.0001172	Paxs	703.26	Joback Method

dvisc	0.0001444	Paxs	660.53	Joback Method
dvisc	0.0001831	Paxs	617.79	Joback Method
dvisc	0.0002406	Paxs	575.06	Joback Method
dvisc	0.0003302	Paxs	532.33	Joback Method
dvisc	0.0004789	Paxs	489.59	Joback Method
dvisc	0.0007459	Paxs	446.86	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=U325647&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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