

Butanal, 2-methyl, 2,4,6-trichlorophenyl hydrazone

Inchi:	InChI=1S/C11H13Cl3N2/c1-3-7(2)6-15-16-11-9(13)4-8(12)5-10(11)14/h4-7,16H,3H2,1-2
InchiKey:	JWQYKPCPUWINQI-GIDUJCDVSA-N
Formula:	C11H13Cl3N2
SMILES:	CCC(C)C=NNc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	279.59

Physical Properties

Property code	Value	Unit	Source
hf	14.94	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	5.091		Crippen Method
mcvol	194.470	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	731.40	K	Joback Method
tc	967.09	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R85095&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

hf:	Enthalpy of formation 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

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