

Butanal, 3-methyl, 2,4,6-trichlorophenyl hydrazone, #1

Inchi: InChI=1S/C11H13Cl3N2/c1-7(2)3-4-15-16-11-9(13)5-8(12)6-10(11)14/h4-7,16H,3H2,1-2H
InchiKey: IZCAZFDUMTUKBT-SYZQJQIISA-N
Formula: C11H13Cl3N2
SMILES: CC(C)CC=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
rinsol	1989.00		NIST Webbook
tb	731.40	K	Joback Method
tc	967.09	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R85102&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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