

Hexanal, 2,4,6-trichlorophenyl hydrazone

Inchi:	InChI=1S/C12H15Cl3N2/c1-2-3-4-5-6-16-17-12-10(14)7-9(13)8-11(12)15/h6-8,17H,2-5H
InchiKey:	LHOUDHVMCMTYLB-UHFFFAOYSA-N
Formula:	C12H15Cl3N2
SMILES:	CCCCC=NNc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	293.62

Physical Properties

Property code	Value	Unit	Source
hf	-0.42	kJ/mol	Joback Method
hvap	69.47	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.625		Crippen Method
mcpvol	208.560	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	754.72	K	Joback Method
tc	982.08	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R85166&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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