

Heptanal, 2,4,6-trichlorophenyl hydrazone

Inchi:	InChI=1S/C13H17Cl3N2/c1-2-3-4-5-6-7-17-18-13-11(15)8-10(14)9-12(13)16/h7-9,18H,2-
InchiKey:	LFHLUQYVTHVZPT-REZTVBANS-A-N
Formula:	C13H17Cl3N2
SMILES:	CCCCCCC=NNc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	307.65

Physical Properties

Property code	Value	Unit	Source
hf	-21.06	kJ/mol	Joback Method
hvap	71.70	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.015		Crippen Method
mcpvol	222.650	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	777.60	K	Joback Method
tc	1001.49	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R85152&Units=SI

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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