

Pentanal, 2,4,6-trichlorophenyl hydrazone, #2

Inchi: InChI=1S/C11H13Cl3N2/c1-2-3-4-5-15-16-11-9(13)6-8(12)7-10(11)14/h5-7,16H,2-4H2,1
InchiKey: PGLKSYVQUISHTE-PJQLUOCWSA-N
Formula: C11H13Cl3N2
SMILES: CCCCC=NNc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 279.59

Physical Properties

Property code	Value	Unit	Source
hf	20.22	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.235		Crippen Method
mcvol	194.470	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	731.84	K	Joback Method
tc	963.16	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R85205&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
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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