2-Hexenal (E), 2,4,6-trichlorophenyl hydrazone, #2

Inchi: InChI=1S/C12H13Cl3N2/c1-2-3-4-5-6-16-17-12-10(14)7-9(13)8-11(12)15/h4-8,17H,2-3H

InchiKey: HYWZYTFTKRTXFT-TUQJRISCSA-N

Formula: C12H13Cl3N2

SMILES: CCCC=CC=NNc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 291.60

Physical Properties

Property code	Value	Unit	Source
hf	116.80	kJ/mol	Joback Method
hvap	69.43	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.401		Crippen Method
mcvol	204.260	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2207.00		NIST Webbook
rinpol	2207.00		NIST Webbook
tb	758.88	K	Joback Method
tc	994.50	K	Joback Method

Sources

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=R85013&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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