

4-Heptanone, 2,4,6-trichlorophenyl hydrazone

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

Physical Properties

Property code	Value	Unit	Source
hf	-30.85	kJ/mol	Joback Method
hvap	71.78	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.015		Crippen Method
mcvol	222.650	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
tb	777.48	K	Joback Method
tc	1004.50	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R85045&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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