

Propanal, 2,4,6-trichlorophenyl hydrazone, #1

Inchi: InChI=1S/C9H9Cl3N2/c1-2-3-13-14-9-7(11)4-6(10)5-8(9)12/h3-5,14H,2H2,1H3/b13-3+
InchiKey: LBBCNSGFIOMURM-QLKAYGNNSA-N
Formula: C9H9Cl3N2
SMILES: CCC=NNc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 251.54

Physical Properties

Property code	Value	Unit	Source
hf	61.50	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.455		Crippen Method
mcvol	166.290	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1846.00		NIST Webbook
tb	686.08	K	Joback Method
tc	926.69	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=R85219&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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