

(Phenylazo)triphenylmethane

Inchi: InChI=1S/C25H20N2/c1-5-13-21(14-6-1)25(22-15-7-2-8-16-22,23-17-9-3-10-18-23)27-26
InchiKey: YFMFSCRSAWIWOP-CYYJNZCTSA-N
Formula: C25H20N2
SMILES: c1ccc(N=NC(c2ccccc2)(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 348.44
CAS: 981-18-0

Physical Properties

Property code	Value	Unit	Source
chs	-13270.00	kJ/mol	NIST Webbook
hf	425.26	kJ/mol	Joback Method
hvap	85.72	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.762		Crippen Method
mcvol	283.730	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
tb	1024.09	K	Joback Method
tc	1320.80	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C981180&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

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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