

ACETALDEHYDE, PHENYLHYDRAZONE

Inchi: InChI=1S/C8H10N2/c1-2-9-10-8-6-4-3-5-7-8/h2-7,10H,1H3
InchiKey: KURBTRNHGDQKOS-UHFFFAOYSA-N
Formula: C8H10N2
SMILES: CC=NNc1ccccc1
Mol. weight [g/mol]: 134.18

Physical Properties

Property code	Value	Unit	Source
af	0.4998		Cheméo Relay (1.0)
chs	-4436.30	kJ/mol	NIST Webbook
gf	308.97	kJ/mol	Cheméo Relay (1.0, beta)
hf	243.93	kJ/mol	Cheméo Relay (1.0)
hfs	-167.00	kJ/mol	NIST Webbook
hfs	-141.00	kJ/mol	NIST Webbook
hvap	61.88	kJ/mol	Cheméo Relay (1.0)
ie	7.85	eV	Cheméo Relay (1.0)
log10ws	-1.19		Cheméo Relay (1.0)
logp	2.104		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	504.16	K	Cheméo Relay (1.0)
tc	757.66	K	Cheméo Relay (1.0)
tf	306.87	K	Cheméo Relay (1.0)

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C935079&Units=SI>

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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