

3-(PHENYLHYDRAZONO)-2-BUTANONE

Other names:	2,3-Butanedione 2-(phenylhydrazone) Biacetyl phenylhydrazone
Inchi:	InChI=1S/C10H12N2O/c1-8(9(2)13)11-12-10-6-4-3-5-7-10/h3-7,12H,1-2H3
InchiKey:	HUHADASXDUCZMY-UHFFFAOYSA-N
Formula:	C10H12N2O
SMILES:	CC(=O)C(C)=NNc1ccccc1
Mol. weight [g/mol]:	176.22

Physical Properties

Property code	Value	Unit	Source
chs	-5677.30	kJ/mol	NIST Webbook
hfs	-0.40	kJ/mol	NIST Webbook
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-1.44		Cheméo Relay (1.0)
logp	2.063		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
tb	556.55	K	Cheméo Relay (1.0)
tf	365.99	K	Cheméo Relay (1.0)

Sources

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=C13732326&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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