

N-[2-(3-methylpyrazyl)]-3-methyl-2-pyrazone

Inchi:	InChI=1S/C10H10N4O/c1-7-9(13-4-3-11-7)14-6-5-12-8(2)10(14)15/h3-6H,1-2H3
InchiKey:	WVKFRXVHSWOVQH-UHFFFAOYSA-N
Formula:	C10H10N4O
SMILES:	Cc1nccnc1-n1ccnc(C)c1=O
Mol. weight [g/mol]:	202.21
CAS:	116373-03-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	0.639		Crippen Method
mcvol	150.030	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373036&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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