4-Nitro-1,3,5-trimethylpyrazole

Other names: 4-Nitro-1,3,5-trimethylpyrazole
Inchi: InChI=1S/C6H9N3O2/c1-4-6(9(10)11)5(2)8(3)7-4/h1-3H3
InchiKey: YSZYFGMARJFMJK-UHFFFAOYSA-N
Formula: C6H9N3O2
SMILES: Cc1nn(C)c(C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 155.16

Physical Properties

Property code	Value	Unit	Source
logp	0.945		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
tf	405.09	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1125300&Units=SI
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

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.