

Nifenazone

Inchi: InChI=1S/C17H16N4O2/c1-12-15(19-16(22)13-7-6-10-18-11-13)17(23)21(20(12)2)14-8-4
InchiKey: BRZANEXCSZCZCI-UHFFFAOYSA-N
Formula: C17H16N4O2
SMILES: Cc1c(NC(=O)c2cccnc2)c(=O)n(-c2ccccc2)n1C
Mol. weight [g/mol]: 308.34

Physical Properties

Property code	Value	Unit	Source
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-2.15		Cheméo Relay (1.0)
logp	2.132		Crippen Method
mcvol	230.770	ml/mol	McGowan Method
tb	689.25	K	Cheméo Relay (1.0)
tf	526.85	K	Cheméo Relay (1.0)

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2139471&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

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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