Amrinone

Inchi: InChI=1S/C10H9N3O/c11-9-5-8(6-13-10(9)14)7-1-3-12-4-2-7/h1-6H,11H2,(H,13,14)
InchiKey: RNLQIBCLLYYYFJ-UHFFFAOYSA-N
Formula: C10H9N3O
SMILES: Nc1cc(-c2ccncc2)c[nH]c1=O
Mol. weight [g/mol]: 187.20
CAS: 60719-84-8

Physical Properties

Property code	Value	Unit	Source
hf	106.90	kJ/mol	Cheméo Relay (1.0)
hvap	117.53	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-1.43		Cheméo Relay (1.0)
logp	0.537		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
tb	648.31	K	Cheméo Relay (1.0)
tf	568.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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