

1-Pentamine, N-nitroso-N-pentyl-

Other names:	1-Pentamine, N-nitroso-N-pentyl- Diamylnitrosamine Dipentylnitrosamine Dipentylnitrosoamine N-Nitrosodi-n-amylamine N-Nitrosodiamylamine N-Nitrosodipentylamine Di-N-amylnitrosamine Di-N-pentylnitrosamine Diamylnitrosamin N-Nitrosodi-N-pentylamine Nitrosodi-N-pentylamine N,N-Dipentylnitrosamine NSC 73601
Inchi:	InChI=1S/C10H22N2O/c1-3-5-7-9-12(11-13)10-8-6-4-2/h3-10H2,1-2H3
InchiKey:	OELWBYBVFOLSTA-UHFFFAOYSA-N
Formula:	C10H22N2O
SMILES:	CCCCCN(CCCCC)N=O
Mol. weight [g/mol]:	186.30

Physical Properties

Property code	Value	Unit	Source
hf	-135.61	kJ/mol	Cheméo Relay (1.0)
hvap	59.52	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
logp	3.350		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
tb	532.18	K	Cheméo Relay (1.0)
tf	275.88	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=C13256069&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>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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