2-UNDECANONE 2,4-DINITROPHENYLHYDRAZONE

Other names: 2,4-dinitrophenylhydrazone 2-undecanone
Inchi: InChI=1S/C17H26N4O4/c1-3-4-5-6-7-8-9-10-14(2)18-19-16-12-11-15(20(22)23)13-17(16
InchiKey: IUEBGTPEQHNPFM-UHFFFAOYSA-N
Formula: C17H26N4O4
SMILES: CCCCCCCCCC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 350.42

Physical Properties

Property code	Value	Unit	Source
logp	5.431		Crippen Method
mcvol	277.130	ml/mol	McGowan Method
rinpol	2988.00		NIST Webbook
rinpol	2988.00		NIST Webbook
tf	370.40	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2121906&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point