

2,4-Dinitrophenylhydrazone of 1-n-pentanesulfonyl-2-propanone

Inchi:	InChI=1S/C14H20N4O6S/c1-3-4-5-8-25(23,24)10-11(2)15-16-13-7-6-12(17(19)20)9-14(1)
InchiKey:	IACUFLAADRECAH-PTNGSMBKSA-N
Formula:	C14H20N4O6S
SMILES:	CCCCCS(=O)(=O)CC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	372.40
CAS:	97172-82-2

Physical Properties

Property code	Value	Unit	Source
hf	-467.67	kJ/mol	Joback Method
hvap	112.00	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	2.896		Crippen Method
mcvol	262.950	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
tb	1034.55	K	Joback Method
tc	1281.56	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97172822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/40-359-9/2-4-Dinitrophenylhydrazone-of-1-n-pentanesulfonyl-2-propanone.pdf>

Generated by Cheméo on 2025-12-05 15:30:32.368647835 +0000 UTC m=+4696829.898688499.

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