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

Inchi: InChI=1S/C15H22N4O6S/c1-3-4-5-6-9-26(24,25)11-12(2)16-17-14-8-7-13(18(20)21)10-1

InchiKey: SHHCSWIFNOVISB-VBKFSLOCSA-N

Formula: C15H22N4O6S

SMILES: CCCCCCS(=O)(=O)CC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]

Mol. weight [g/mol]: 386.42

CAS: 97498-49-2

Physical Properties

Property code	Value	Unit	Source
hf	-488.31	kJ/mol	Joback Method
hvap	114.23	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	3.286		Crippen Method
mcvol	277.040	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
tb	1057.43	K	Joback Method
tc	1304.51	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97498492&Units=SI

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

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