

3,5-Dinitrosalicylaldehyde

Other names:	3,5-Dinitro-2-hydroxybenzaldehyde Benzaldehyde, 2-hydroxy-3,5-dinitro-
Inchi:	InChI=1S/C7H4N2O6/c10-3-4-1-5(8(12)13)2-6(7(4)11)9(14)15/h1-3,11H
InchiKey:	FLJXIBHYDIMYRS-UHFFFAOYSA-N
Formula:	C7H4N2O6
SMILES:	O=Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Mol. weight [g/mol]:	212.12
CAS:	2460-59-5

Physical Properties

Property code	Value	Unit	Source
gf	-81.83	kJ/mol	Joback Method
hf	-258.63	kJ/mol	Joback Method
hfus	37.94	kJ/mol	Joback Method
hvap	87.69	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	1.021		Crippen Method
mcvol	128.010	ml/mol	McGowan Method
pc	5552.58	kPa	Joback Method
tb	829.16	K	Joback Method
tc	1106.41	K	Joback Method
tf	661.05	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.50	J/mol×K	829.16	Joback Method
cpg	344.40	J/mol×K	875.37	Joback Method
cpg	350.92	J/mol×K	921.58	Joback Method
cpg	357.21	J/mol×K	967.79	Joback Method
cpg	363.39	J/mol×K	1013.99	Joback Method
cpg	369.58	J/mol×K	1060.20	Joback Method
cpg	375.92	J/mol×K	1106.41	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=C2460595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/29-276-4/3-5-Dinitrosalicylaldehyde.pdf>

Generated by Cheméo on 2025-12-05 13:57:36.68598924 +0000 UTC m=+4691254.216029902.

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