

2,4-Dinitrophenol, isoBOC

Inchi:	InChI=1S/C11H12N2O7/c1-7(2)6-19-11(14)20-10-4-3-8(12(15)16)5-9(10)13(17)18/h3-5,7
InchiKey:	LUNFMISJQDNGJE-UHFFFAOYSA-N
Formula:	C11H12N2O7
SMILES:	CC(C)COC(=O)Oc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	284.22

Physical Properties

Property code	Value	Unit	Source
gf	-135.37	kJ/mol	Joback Method
hf	-460.60	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	2.674		Crippen Method
mcvol	190.240	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	2021.00		NIST Webbook
rinpol	2021.00		NIST Webbook
tb	889.67	K	Joback Method
tc	1140.97	K	Joback Method
tf	631.80	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.65	J/mol×K	889.67	Joback Method
cpg	568.22	J/mol×K	931.55	Joback Method
cpg	576.57	J/mol×K	973.44	Joback Method
cpg	583.71	J/mol×K	1015.32	Joback Method
cpg	589.66	J/mol×K	1057.20	Joback Method
cpg	594.40	J/mol×K	1099.09	Joback Method
cpg	597.96	J/mol×K	1140.97	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=R234967&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
hvpap:	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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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