

3,5-Dinitrophenol

Inchi:	InChI=1S/C6H4N2O5/c9-6-2-4(7(10)11)1-5(3-6)8(12)13/h1-3,9H
InchiKey:	UEMBNLWZFIWQFL-UHFFFAOYSA-N
Formula:	C6H4N2O5
SMILES:	O=[N+]([O-])c1cc(O)cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	184.11
CAS:	586-11-8

Physical Properties

Property code	Value	Unit	Source
gf	18.90	kJ/mol	Joback Method
hf	-140.94	kJ/mol	Joback Method
hfus	33.45	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.209		Crippen Method
mcvol	112.350	ml/mol	McGowan Method
pc	5871.90	kPa	Joback Method
tb	752.64	K	Joback Method
tc	1038.65	K	Joback Method
tf	399.10	K	NIST Webbook
tf	399.10 ± 0.20	K	NIST Webbook
vc	0.394	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.91	J/mol×K	752.64	Joback Method
cpg	295.32	J/mol×K	800.31	Joback Method
cpg	302.18	J/mol×K	847.98	Joback Method
cpg	308.65	J/mol×K	895.64	Joback Method
cpg	314.88	J/mol×K	943.31	Joback Method
cpg	321.02	J/mol×K	990.98	Joback Method
cpg	327.23	J/mol×K	1038.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C586118&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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