Benzenethiol, 4-nitro-

Other names:	p-Nitrothiophenol
	p-Nitrophenyl mercaptan
	p-Nitrobenzenethiol
	Benzenethiol, p-nitro-
	4-Nitrobenzenethiol
	4-Nitrothiophenol
Inchi:	InChI=1S/C6H5NO2S/c8-7(9)5-1-3-6(10)4-2-5/h1-4,10H
InchiKey:	AXBVSRMHOPMXBA-UHFFFAOYSA-N
Formula:	C6H5NO2S
SMILES:	O=[N+]([O-])c1ccc(S)cc1
Mol. weight [g/mol]:	155.17
CAS:	1849-36-1

Physical Properties

Property code	Value	Unit	Source
gf	167.36	kJ/mol	Joback Method
hf	85.61	kJ/mol	Joback Method
hfus	20.35	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	1.884		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	583.04	K	Joback Method
tc	861.59	K	Joback Method
tf	376.39	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.05	J/mol×K	583.04	Joback Method
cpg	227.87	J/mol×K	629.46	Joback Method
cpg	236.80	J/mol×K	675.89	Joback Method

cpg	244.91	J/mol×K	722.31	Joback Method
cpg	252.23	J/mol×K	768.74	Joback Method
cpg	258.83	J/mol×K	815.16	Joback Method
cpg	264.75	J/mol×K	861.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1849361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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