Methyl 4-nitrophenyl sulphide

Other names:	4-Nitrothioanisole
	Benzene, 1-(methylthio)-4-nitro-
Inchi:	InChI=1S/C7H7NO2S/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3
InchiKey:	NEZGPRYOJVPJKL-UHFFFAOYSA-N
Formula:	C7H7NO2S
SMILES:	CSc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	169.20
CAS:	701-57-5

Physical Properties

Property code	Value	Unit	Source
gf	179.51	kJ/mol	Joback Method
hf	68.36	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	57.52	kJ/mol	Joback Method
ie	8.59 ± 0.01	eV	NIST Webbook
log10ws	-2.87		Crippen Method
logp	2.317		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	611.84	K	Joback Method
tc	882.47	K	Joback Method
tf	385.60	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.24	J/mol×K	611.84	Joback Method
cpg	275.36	J/mol×K	656.95	Joback Method
cpg	285.55	J/mol×K	702.05	Joback Method
cpg	294.82	J/mol×K	747.16	Joback Method
cpg	303.23	J/mol×K	792.26	Joback Method
cpg	310.80	J/mol×K	837.37	Joback Method

cpg	317.57	J/mol×K	882.47	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=C701575&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
ie:	Ionization energy
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