

4-Nitrobenzyl thiocyanate

Other names:	p-Nitrobenzylthiocyanate Thiocyanic acid, (4-nitrophenyl)methyl ester Thiocyanic acid, (p-nitrobenzyl) ester Thiocyanic acid, 4-nitrobenzyl ester
Inchi:	InChI=1S/C8H6N2O2S/c9-6-13-5-7-1-3-8(4-2-7)10(11)12/h1-4H,5H2
InchiKey:	NUMYTLIHYKESKM-UHFFFAOYSA-N
Formula:	C8H6N2O2S
SMILES:	N#CSCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	194.21
CAS:	13287-49-5

Physical Properties

Property code	Value	Unit	Source
gf	321.11	kJ/mol	Joback Method
hf	212.60	kJ/mol	Joback Method
hfus	27.13	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.309		Crippen Method
mcvol	134.970	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	736.80	K	Joback Method
tc	1011.26	K	Joback Method
tf	461.86	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.34	J/molxK	736.80	Joback Method
cpg	329.24	J/molxK	782.54	Joback Method
cpg	337.22	J/molxK	828.29	Joback Method
cpg	344.34	J/molxK	874.03	Joback Method
cpg	350.64	J/molxK	919.77	Joback Method

cpg	356.14	J/mol×K	965.52	Joback Method
cpg	360.89	J/mol×K	1011.26	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13287495&Units=SI

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
hvp:	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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