Phenetole, 4-chloro-2-nitro

Other names: Benzene, 4-chloro-1-ethoxy-2-nitro
Inchi: InChI=1S/C8H8ClNO3/c1-2-13-8-4-3-6(9)5-7(8)10(11)12/h3-5H,2H2,1H3
InchiKey: SKMDJPLCXWZTCN-UHFFFAOYSA-N
Formula: C8H8ClNO3
SMILES: CCOc1ccc(Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 201.61
CAS: 102236-24-8

Physical Properties

Property code	Value	Unit	Source
gf	28.25	kJ/mol	Joback Method
hf	-153.58	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	60.39	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.647		Crippen Method
mcvol	135.350	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	630.77	K	Joback Method
tc	875.97	K	Joback Method
tf	427.14	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.81	J/mol×K	630.77	Joback Method
cpg	319.68	J/mol×K	671.64	Joback Method
cpg	329.78	J/mol×K	712.50	Joback Method
cpg	339.13	J/mol×K	753.37	Joback Method
cpg	347.75	J/mol×K	794.23	Joback Method
cpg	355.64	J/mol×K	835.10	Joback Method
cpg	362.83	J/mol×K	875.97	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=C102236248&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