Phenol, 2,5-dimethyl-4-nitro-

Inchi: InChI=1S/C8H9NO3/c1-5-4-8(10)6(2)3-7(5)9(11)12/h3-4,10H,1-2H3
InchiKey: DSWZKAODNLLINU-UHFFFAOYSA-N
Formula: C8H9NO3
SMILES: Cc1cc([N+](=O)[O-])c(C)cc1O
Mol. weight [g/mol]: 167.16
CAS: 3139-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-9.44	kJ/mol	Joback Method
hf	-182.93	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.917		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	651.54	K	Joback Method
tc	906.38	K	Joback Method
tf	486.71	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.80	J/mol×K	651.54	Joback Method
cpg	317.13	J/mol×K	694.01	Joback Method
cpg	326.73	J/mol×K	736.49	Joback Method
cpg	335.71	J/mol×K	778.96	Joback Method
cpg	344.15	J/mol×K	821.43	Joback Method
cpg	352.17	J/mol×K	863.91	Joback Method

cpg	359.86	J/mol×K	906.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3139057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume