Phenol, 2,4-dinitro-6-ethyl-

Inchi: InChI=1S/C8H8N2O5/c1-2-5-3-6(9(12)13)4-7(8(5)11)10(14)15/h3-4,11H,2H2,1H3
InchiKey: SYWMIOFIFBKHTK-UHFFFAOYSA-N
Formula: C8H8N2O5
SMILES: CCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Mol. weight [g/mol]: 212.16
CAS: 4099-71-2

Physical Properties

Property code	Value	Unit	Source
gf	26.11	kJ/mol	Joback Method
hf	-193.69	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
ie	9.98 ± 0.08	eV	NIST Webbook
log10ws	-3.12		Crippen Method
logp	1.771		Crippen Method
mcvol	140.530	ml/mol	McGowan Method
pc	4374.18	kPa	Joback Method
tb	803.38	K	Joback Method
tc	1075.70	K	Joback Method
tf	630.32	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.59	J/mol×K	803.38	Joback Method
cpg	394.79	J/mol×K	848.77	Joback Method
cpg	403.46	J/mol×K	894.15	Joback Method
cpg	411.73	J/mol×K	939.54	Joback Method
cpg	419.72	J/mol×K	984.92	Joback Method
cpg	427.56	J/mol×K	1030.31	Joback Method
cpg	435.39	J/mol×K	1075.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4099712&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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