2,4-Dinitro-N-ethylaniline

Other names: Benzenamine, N-ethyl-2,4-dinitro-
N-ethyl-2,4-dinitroaniline
Inchi: InChI=1S/C8H9N3O4/c1-2-9-7-4-3-6(10(12)13)5-8(7)11(14)15/h3-5,9H,2H2,1H3
InchiKey: YYOUTZBUOQBAAE-UHFFFAOYSA-N
Formula: C8H9N3O4
SMILES: CCNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 211.17
CAS: 3846-50-2

Physical Properties

Property code	Value	Unit	Source
gf	270.12	kJ/mol	Joback Method
hf	37.09	kJ/mol	Joback Method
hfus	37.56	kJ/mol	Joback Method
hvap	76.62	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	1.935		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	772.93	K	Joback Method
tc	1035.37	K	Joback Method
tf	571.26	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.67	J/mol×K	772.93	Joback Method
cpg	403.82	J/mol×K	816.67	Joback Method
cpg	413.03	J/mol×K	860.41	Joback Method
cpg	421.36	J/mol×K	904.15	Joback Method
cpg	428.86	J/mol×K	947.89	Joback Method
cpg	435.60	J/mol×K	991.63	Joback Method
cpg	441.61	J/mol×K	1035.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3846502&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume