N-ETHYL-2,4-DINITROANILINE

Other names: 2,4-dinitro-N-ethylaniline
Benzenamine, N-ethyl-2,4-dinitro-
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]: 211.18

Physical Properties

Property code	Value	Unit	Source
hf	34.23	kJ/mol	Cheméo Relay (1.0)
hfus	19.67	kJ/mol	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
hvap	80.50	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-3.43		Cheméo Relay (1.0)
logp	1.935		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
tb	568.44	K	Cheméo Relay (1.0)
tf	384.86	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures:	https://www.doi.org/10.1016/j.jct.2010.03.025
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3846502&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point