Benzenamine, 2,4-dinitro-N-propyl-

Other names: Aniline, 2,4-dinitro-N-propyl-
Inchi: InChI=1S/C9H11N3O4/c1-2-5-10-8-4-3-7(11(13)14)6-9(8)12(15)16/h3-4,6,10H,2,5H2,1H
InchiKey: VTYSAZUSTIWCND-UHFFFAOYSA-N
Formula: C9H11N3O4
SMILES: CCCNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 225.20
CAS: 13059-84-2

Physical Properties

Property code	Value	Unit	Source
gf	278.54	kJ/mol	Joback Method
hf	16.45	kJ/mol	Joback Method
hfus	40.15	kJ/mol	Joback Method
hvap	78.85	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.325		Crippen Method
mcvol	158.730	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	795.81	K	Joback Method
tc	1052.39	K	Joback Method
tf	582.53	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.33	J/mol×K	795.81	Joback Method
cpg	456.06	J/mol×K	838.57	Joback Method
cpg	465.83	J/mol×K	881.34	Joback Method
cpg	474.70	J/mol×K	924.10	Joback Method
cpg	482.72	J/mol×K	966.86	Joback Method
cpg	489.96	J/mol×K	1009.63	Joback Method
cpg	496.46	J/mol×K	1052.39	Joback Method

Sources

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=C13059842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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