Naphthalene, 1,3-dinitro-

Other names: 1,3-Dinitronaphthalene
2,6-Dinitro-9H-fluoren-9-one
Inchi: InChI=1S/C10H6N2O4/c13-11(14)8-5-7-3-1-2-4-9(7)10(6-8)12(15)16/h1-6H
InchiKey: ULALSFRIGPMWRS-UHFFFAOYSA-N
Formula: C10H6N2O4
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c2ccccc2c1
Mol. weight [g/mol]: 218.17
CAS: 606-37-1

Physical Properties

Property code	Value	Unit	Source
ea	1.98 ± 0.05	eV	NIST Webbook
ea	1.78 ± 0.10	eV	NIST Webbook
gf	304.22	kJ/mol	Joback Method
hf	133.41	kJ/mol	Joback Method
hfus	34.66	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	2.656		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
rinpol	332.75		NIST Webbook
rinpol	334.60		NIST Webbook
tb	787.50	K	Joback Method
tc	1073.68	K	Joback Method
tf	573.84	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.77	J/mol×K	787.50	Joback Method
cpg	385.35	J/mol×K	835.20	Joback Method
cpg	394.02	J/mol×K	882.89	Joback Method

cpg	401.92	J/mol×K	930.59	Joback Method
cpg	409.18	J/mol×K	978.29	Joback Method
cpg	415.93	J/mol×K	1025.98	Joback Method
cpg	422.31	J/mol×K	1073.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C606371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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