3-nitrophthalonitrile

Other names: 3-nitro-1,2-benzenedicarbonitrile
Inchi: InChI=1S/C8H3N3O2/c9-4-6-2-1-3-8(11(12)13)7(6)5-10/h1-3H
InchiKey: UZJZIZFCQFZDHP-UHFFFAOYSA-N
Formula: C8H3N3O2
SMILES: N#Cc1cccc([N+](=O)[O-])c1C#N
Mol. weight [g/mol]: 173.13

Physical Properties

Property code	Value	Unit	Source
gf	411.54	kJ/mol	Joback Method
hf	324.14	kJ/mol	Joback Method
hfus	19.20	kJ/mol	Solubility and Solution Thermodynamics of 3-Nitrophthalonitrile in 12 Neat Solvents at Temperatures from 278.15 to 323.15 K
hvap	74.55	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.338		Crippen Method
mcvol	120.000	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	775.08	K	Joback Method
tc	1043.50	K	Joback Method
tf	504.97	K	Joback Method
tt	435.55	K	Solubility and Solution Thermodynamics of 3-Nitrophthalonitrile in 12 Neat Solvents at Temperatures from 278.15 to 323.15 K
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.31	J/mol×K	775.08	Joback Method

cpg	286.77	J/mol×K	819.82	Joback Method
cpg	292.58	J/mol×K	864.55	Joback Method
cpg	297.79	J/mol×K	909.29	Joback Method
cpg	302.43	J/mol×K	954.03	Joback Method
cpg	306.53	J/mol×K	998.77	Joback Method
cpg	310.14	J/mol×K	1043.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and Solution Thermodynamics of 3-Nitrophthalonitrile in 12 Neat Solvents at Temperatures from 278.15 to 323.15 K:	https://www.doi.org/10.1021/acs.jced.8b01250
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
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
tt:	Triple Point Temperature
vc:	Critical Volume