1-tert-Butyl-3-nitrobenzene

Other names: Benzene, 1-(1,1-dimethylethyl)-3-nitro-
Inchi: InChI=1S/C10H13NO2/c1-10(2,3)8-5-4-6-9(7-8)11(12)13/h4-7H,1-3H3
InchiKey: ZKRDQLBHUZNPGZ-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CC(C)(C)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 179.22
CAS: 23132-52-7

Physical Properties

Property code	Value	Unit	Source
gf	174.49	kJ/mol	Joback Method
hf	-44.18	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	56.09	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.892		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	608.47	K	Joback Method
tc	858.26	K	Joback Method
tf	387.43	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.51	J/mol×K	608.47	Joback Method
cpg	376.25	J/mol×K	650.10	Joback Method
cpg	389.79	J/mol×K	691.73	Joback Method
cpg	402.22	J/mol×K	733.36	Joback Method
cpg	413.64	J/mol×K	775.00	Joback Method
cpg	424.12	J/mol×K	816.63	Joback Method
cpg	433.75	J/mol×K	858.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	524.20	K	93.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49917e+01
Coeff. B	-4.55860e+03
Coeff. C	-8.76980e+01
Temperature range (K), min.	397.72
Temperature range (K), max.	558.62

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23132527&Units=SI

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume