1-TERT-BUTYL-2-NITROBENZENE

Other names: Benzene, 1-(1,1-dimethylethyl)-2-nitro-
1-tert-Butyl-4-nitrobenzene
Inchi: InChI=1S/C10H13NO2/c1-10(2,3)8-6-4-5-7-9(8)11(12)13/h4-7H,1-3H3
InchiKey: IWTHGPTVKBEURV-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CC(C)(C)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
hf	-31.81	kJ/mol	Cheméo Relay (1.0)
hfus	19.26	kJ/mol	Joback Method
hvap	65.00 ± 0.60	kJ/mol	NIST Webbook
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-4.09		Cheméo Relay (1.0)
logp	2.892		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
tb	527.07	K	Cheméo Relay (1.0)
tf	292.58	K	Cheméo Relay (1.0)

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
hvapt	64.80 ± 0.60	kJ/mol	300.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.70	K	102.00	NIST Webbook
tbrp	387.70	K	1.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1886573&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

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
hvapt: Enthalpy of vaporization at a given temperature
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
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point