BENZENE, 1,3,5-TRIMETHYL-2-NITRO-

Other names:	1,3,5-Trimethyl-2-nitrobenzene
	2,4,6-Trimethyl-1-nitrobenzene
	2,4,6-Trimethylnitrobenzene
	2-Nitromesitylene
	Mesitylene, 2-nitro-
	Mononitromesitylene
	NSC 5413
	Nitromesitylene
Inchi:	InChI=1S/C9H11NO2/c1-6-4-7(2)9(10(11)12)8(3)5-6/h4-5H,1-3H3
InchiKey:	SCEKDQTVGHRSNS-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	Cc1cc(C)c([N+](=O)[O-])c(C)c1
Mol. weight [g/mol]:	165.19
CAS:	603-71-4

Physical Properties

Property code	Value	Unit	Source
af	0.5417		Cheméo Relay (1.0)
affp	823.80	kJ/mol	NIST Webbook
basg	793.10	kJ/mol	NIST Webbook
chs	-5008.20 ± 1.60	kJ/mol	NIST Webbook
ea	0.71 ± 0.09	eV	NIST Webbook
ea	0.78 ± 0.05	eV	NIST Webbook
ea	0.71 ± 0.10	eV	NIST Webbook
ea	0.70 ± 0.10	eV	NIST Webbook
gf	143.97	kJ/mol	Joback Method
hf	-26.80 ± 2.20	kJ/mol	NIST Webbook
hfs	-105.40 ± 2.00	kJ/mol	NIST Webbook
hfus	23.30	kJ/mol	Joback Method
hsub	78.60 ± 1.00	kJ/mol	NIST Webbook
hsub	78.60 ± 1.00	kJ/mol	NIST Webbook
hvap	62.74	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	NIST Webbook
ie	9.01	eV	NIST Webbook
log10ws	-3.54		Cheméo Relay (1.0)
logp	2.520		Crippen Method
mcvol	131.330	ml/mol	McGowan Method

pc	3142.03	kPa	Joback Method
tb	528.20	K	NIST Webbook
tc	770.50	K	Cheméo Relay (1.0)
tf	317.00 ± 1.50	K	NIST Webbook
vc	0.464	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.91	J/mol×K	598.78	Joback Method
cpg	321.55	J/mol×K	639.04	Joback Method
cpg	333.39	J/mol×K	679.30	Joback Method
cpg	344.46	J/mol×K	719.56	Joback Method
cpg	354.78	J/mol×K	759.82	Joback Method
cpg	364.37	J/mol×K	800.08	Joback Method
cpg	373.27	J/mol×K	840.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49891e+01
Coeff. B	-4.56548e+03
Coeff. C	-8.79760e+01
Temperature range (K), min.	398.52
Temperature range (K), max.	559.73

Sources

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):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603714&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume