2,4,6-TRI-t-BUTYLNITROBENZENE

Other names: 2,4,6-tri-t-Butylnitrobenzene
Benzene, 1,3,5-tris(1,1-dimethylethyl)-2-nitro-
Nitrobenzene, 2,4,6-tri-tert-butyl-
1,3,5-tri(tert-butyl)-2-nitrobenzene
Inchi: InChI=1S/C18H29NO2/c1-16(2,3)12-10-13(17(4,5)6)15(19(20)21)14(11-12)18(7,8)9/h10-
InchiKey: IMDZOFHRUMJNQR-UHFFFAOYSA-N
Formula: C18H29NO2
SMILES: CC(C)(C)c1cc(C(C)(C)C)c([N+](=O)[O-])c(C(C)(C)C)c1
Mol. weight [g/mol]: 291.43

Physical Properties

Property code	Value	Unit	Source
chs	-10942.10 ± 3.20	kJ/mol	NIST Webbook
hf	-189.90 ± 4.40	kJ/mol	NIST Webbook
hfs	-271.30 ± 4.00	kJ/mol	NIST Webbook
hfus	24.37	kJ/mol	Joback Method
hsub	96.40 ± 1.00	kJ/mol	NIST Webbook
hsub	81.40 ± 1.80	kJ/mol	NIST Webbook
hsub	81.40 ± 1.80	kJ/mol	NIST Webbook
hvap	79.53	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	NIST Webbook
log10ws	-6.86		Cheméo Relay (1.0)
logp	5.487		Crippen Method
mcvol	258.140	ml/mol	McGowan Method
tb	569.62	K	Cheméo Relay (1.0)
tf	369.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.47	J/mol×K	795.01	Joback Method
cpg	806.80	J/mol×K	834.77	Joback Method
cpg	823.86	J/mol×K	874.53	Joback Method
cpg	839.78	J/mol×K	914.29	Joback Method

cpg	854.72	J/mol×K	954.04	Joback Method
cpg	868.82	J/mol×K	993.80	Joback Method
cpg	882.23	J/mol×K	1033.56	Joback Method
hfust	19.25	kJ/mol	482.80	NIST Webbook
hsubt	94.80 ± 1.00	kJ/mol	350.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4074253&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point