2,4,6 Tri-tert-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
CAS:	4074-25-3

Physical Properties

Property code	Value	Unit	Source
gf	228.27	kJ/mol	Joback Method
hf	-249.74	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.487		Crippen Method
mcvol	258.140	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
tb	795.01	K	Joback Method
tc	1033.56	K	Joback Method
tf	507.47	K	Joback Method
vc	0.985	m3/kmol	Joback Method

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

Sources

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=C4074253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
vc:	Critical Volume