

2,5-di-tert-Butylnitrobenzene

Inchi:	InChI=1S/C14H21NO2/c1-13(2,3)10-7-8-11(14(4,5)6)12(9-10)15(16)17/h7-9H,1-6H3
InchiKey:	LXBUSXRSPLOXCP-UHFFFAOYSA-N
Formula:	C14H21NO2
SMILES:	CC(C)(C)c1ccc(C(C)(C)C)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	235.32
CAS:	3463-35-2

Physical Properties

Property code	Value	Unit	Source
gf	201.38	kJ/mol	Joback Method
hf	-146.96	kJ/mol	Joback Method
hfus	21.81	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.190		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
tb	701.74	K	Joback Method
tc	945.60	K	Joback Method
tf	447.45	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.24	J/molxK	701.74	Joback Method
cpg	583.38	J/molxK	742.38	Joback Method
cpg	599.20	J/molxK	783.03	Joback Method
cpg	613.81	J/molxK	823.67	Joback Method
cpg	627.34	J/molxK	864.31	Joback Method
cpg	639.90	J/molxK	904.95	Joback Method
cpg	651.61	J/molxK	945.60	Joback Method

Sources

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=C3463352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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