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]: 235.33

Physical Properties

Property code	Value	Unit	Source
hf	-133.01	kJ/mol	Cheméo Relay (1.0)
hfus	21.81	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
logp	4.190		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
tb	551.56	K	Cheméo Relay (1.0)
tf	341.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3463352&Units=SI

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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point