Pentamethylnitrobenzene

Inchi: InChI=1S/C11H15NO2/c1-6-7(2)9(4)11(12(13)14)10(5)8(6)3/h1-5H3
InchiKey: RBDSUVKUGRWOPC-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: Cc1c(C)c(C)c([N+](=O)[O-])c(C)c1C
Mol. weight [g/mol]: 193.24
CAS: 13171-59-0

Physical Properties

Property code	Value	Unit	Source
gf	141.55	kJ/mol	Joback Method
hf	-101.95	kJ/mol	Joback Method
hfus	27.70	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.137		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
tb	654.50	K	Joback Method
tc	888.06	K	Joback Method
tf	427.00 ± 2.00	K	NIST Webbook
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.01	J/mol×K	654.50	Joback Method
cpg	416.89	J/mol×K	693.43	Joback Method
cpg	429.97	J/mol×K	732.35	Joback Method
cpg	442.26	J/mol×K	771.28	Joback Method
cpg	453.78	J/mol×K	810.21	Joback Method
cpg	464.54	J/mol×K	849.13	Joback Method
cpg	474.55	J/mol×K	888.06	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=C13171590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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