4-Methyl-3-nitrobenzaldehyde

Other names: Benzaldehyde, 4-methyl-3-nitro-
4-Methyl-3-nitrobenzaldehyde
3-nitro-p-tolualdehyde
Inchi: InChI=1S/C8H7NO3/c1-6-2-3-7(5-10)4-8(6)9(11)12/h2-5H,1H3
InchiKey: KHWGAWBXQOKXIJ-UHFFFAOYSA-N
Formula: C8H7NO3
SMILES: Cc1ccc(C=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 165.15

Physical Properties

Property code	Value	Unit	Source
hf	-81.33	kJ/mol	Cheméo Relay (1.0)
hfus	23.39	kJ/mol	Joback Method
hvap	67.70	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-2.33		Cheméo Relay (1.0)
logp	1.716		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
tb	547.63	K	Cheméo Relay (1.0)
tc	815.62	K	Cheméo Relay (1.0)
tf	314.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.16	J/mol×K	619.58	Joback Method
cpg	286.40	J/mol×K	660.77	Joback Method
cpg	295.87	J/mol×K	701.96	Joback Method
cpg	304.60	J/mol×K	743.15	Joback Method
cpg	312.63	J/mol×K	784.34	Joback Method
cpg	319.99	J/mol×K	825.53	Joback Method
cpg	326.71	J/mol×K	866.72	Joback Method

Sources

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=C31680076&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point