1,2,4-trimethyl-5-nitrobenzene

Inchi: InChI=1S/C9H11NO2/c1-6-4-8(3)9(10(11)12)5-7(6)2/h4-5H,1-3H3
InchiKey: WILMQVBUVCETSB-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: Cc1cc(C)c([N+](=O)[O-])cc1C
Mol. weight [g/mol]: 165.19
CAS: 610-91-3

Physical Properties

Property code	Value	Unit	Source
af	0.5491		Cheméo Relay (1.0)
gf	143.97	kJ/mol	Joback Method
hf	-27.35	kJ/mol	Cheméo Relay (1.0)
hfus	23.30	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-3.59		Cheméo Relay (1.0)
logp	2.520		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	535.01	K	Cheméo Relay (1.0)
tc	776.75	K	Cheméo Relay (1.0)
tf	343.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.91	J/mol×K	598.78	Joback Method
cpg	321.55	J/mol×K	639.04	Joback Method
cpg	333.39	J/mol×K	679.30	Joback Method
cpg	344.46	J/mol×K	719.56	Joback Method
cpg	354.78	J/mol×K	759.82	Joback Method
cpg	364.37	J/mol×K	800.08	Joback Method
cpg	373.27	J/mol×K	840.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51651e+01
Coeff. B	-4.69779e+03
Coeff. C	-9.07560e+01
Temperature range (K), min.	406.52
Temperature range (K), max.	567.51

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point