Anisole, 3,5-dimethyl-2-nitro-

Inchi: InChI=1S/C9H11NO3/c1-6-4-7(2)9(10(11)12)8(5-6)13-3/h4-5H,1-3H3
InchiKey: GUFYOIXUHUNERH-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: COc1cc(C)cc(C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 181.19
CAS: 18102-38-0

Physical Properties

Property code	Value	Unit	Source
gf	38.97	kJ/mol	Joback Method
hf	-169.95	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	58.89	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.220		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	621.20	K	Joback Method
tc	859.07	K	Joback Method
tf	421.01	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.99	J/mol×K	621.20	Joback Method
cpg	344.46	J/mol×K	660.84	Joback Method
cpg	356.17	J/mol×K	700.49	Joback Method
cpg	367.13	J/mol×K	740.13	Joback Method
cpg	377.35	J/mol×K	779.78	Joback Method
cpg	386.83	J/mol×K	819.42	Joback Method
cpg	395.57	J/mol×K	859.07	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=C18102380&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