Benzonitrile, 2,3-dimethoxy-

Other names: o-Veratronitrile
2,3-Dimethoxybenzonitrile
Inchi: InChI=1S/C9H9NO2/c1-11-8-5-3-4-7(6-10)9(8)12-2/h3-5H,1-2H3
InchiKey: LBXGBNHUNHWYRM-UHFFFAOYSA-N
Formula: C9H9NO2
SMILES: COc1cccc(C#N)c1OC
Mol. weight [g/mol]: 163.17
CAS: 5653-62-3

Physical Properties

Property code	Value	Unit	Source
gf	41.23	kJ/mol	Joback Method
hf	-115.06	kJ/mol	Joback Method
hfus	16.21	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.575		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	588.88	K	Joback Method
tc	812.66	K	Joback Method
tf	352.10	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.62	J/mol×K	588.88	Joback Method
cpg	297.31	J/mol×K	626.18	Joback Method
cpg	307.47	J/mol×K	663.47	Joback Method
cpg	317.07	J/mol×K	700.77	Joback Method
cpg	326.11	J/mol×K	738.07	Joback Method
cpg	334.58	J/mol×K	775.36	Joback Method
cpg	342.45	J/mol×K	812.66	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=C5653623&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