1,4-Dimethoxy-2-nitrobenzene

Inchi: InChI=1S/C8H9NO4/c1-12-6-3-4-8(13-2)7(5-6)9(10)11/h3-5H,1-2H3
InchiKey: UPTOWXNJLZJTGD-UHFFFAOYSA-N
Formula: C8H9NO4
SMILES: COc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 183.16

Physical Properties

Property code	Value	Unit	Source
gf	-64.82	kJ/mol	Joback Method
hf	-270.06	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	58.41	kJ/mol	Joback Method
log10ws	-3.12		Aqueous Solubility Prediction Method
logp	1.612		Crippen Method
mcvol	128.980	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	615.76	K	Joback Method
tc	854.02	K	Joback Method
tf	344.90	K	Aqueous Solubility Prediction Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.07	J/mol×K	615.76	Joback Method
cpg	320.70	J/mol×K	655.47	Joback Method
cpg	331.62	J/mol×K	695.18	Joback Method
cpg	341.82	J/mol×K	734.89	Joback Method
cpg	351.29	J/mol×K	774.60	Joback Method
cpg	360.02	J/mol×K	814.31	Joback Method
cpg	368.00	J/mol×K	854.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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