

3,4-Dimethoxy-«beta»-nitrostyrene

Other names:	Ethylene, 1-[3,4-(dimethoxy)phenyl]-2-nitro-
Inchi:	InChI=1S/C10H11NO4/c1-14-9-4-3-8(5-6-11(12)13)7-10(9)15-2/h3-7H,1-2H3/b6-5+
InchiKey:	SYJMYDMKPSZMSB-AATRIKPKSA-N
Formula:	C10H11NO4
SMILES:	COc1ccc(C=C[N+](=O)[O-])cc1OC
Mol. weight [g/mol]:	209.20
CAS:	4230-93-7

Physical Properties

Property code	Value	Unit	Source
gf	32.24	kJ/mol	Joback Method
hf	-194.12	kJ/mol	Joback Method
hfus	28.86	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	1.951		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
tb	665.68	K	Joback Method
tc	904.06	K	Joback Method
tf	436.91	K	Joback Method
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.02	J/mol×K	665.68	Joback Method
cpg	395.61	J/mol×K	705.41	Joback Method
cpg	407.33	J/mol×K	745.14	Joback Method
cpg	418.22	J/mol×K	784.87	Joback Method
cpg	428.29	J/mol×K	824.60	Joback Method
cpg	437.54	J/mol×K	864.33	Joback Method
cpg	446.01	J/mol×K	904.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4230937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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