

Styrene, «beta»-nitro-, (E)-

Other names:	trans-«beta»-Nitrostyrene Benzene, (2-nitroethenyl)-, (E)-
Inchi:	InChI=1S/C8H7NO2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H/b7-6+
InchiKey:	PIAOLBVUVDXHHL-VOTSOKGWSA-N
Formula:	C8H7NO2
SMILES:	O=[N+]([O-])C=Cc1ccccc1
Mol. weight [g/mol]:	149.15
CAS:	5153-67-3

Physical Properties

Property code	Value	Unit	Source
gf	244.66	kJ/mol	Joback Method
hf	134.54	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.934		Crippen Method
mvol	112.940	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	528.20	K	NIST Webbook
tc	820.37	K	Joback Method
tf	344.87	K	Joback Method
vc	0.438	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.26	J/mol×K	565.12	Joback Method
cpg	258.06	J/mol×K	607.66	Joback Method
cpg	268.84	J/mol×K	650.20	Joback Method
cpg	278.67	J/mol×K	692.75	Joback Method
cpg	287.64	J/mol×K	735.29	Joback Method
cpg	295.84	J/mol×K	777.83	Joback Method
cpg	303.34	J/mol×K	820.37	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5153673&Units=SI

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
h vap:	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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