

4-Methyl-«beta»-methyl-«beta»-nitrostyrene

Other names:	trans-4-Methyl-«beta»-methyl-«beta»-nitrostyrene
Inchi:	InChI=1S/C10H11NO2/c1-8-3-5-10(6-4-8)7-9(2)11(12)13/h3-7H,1-2H3/b9-7-
InchiKey:	JEKFDNFWPBWEKO-CLFYBASSA-N
Formula:	C10H11NO2
SMILES:	<chem>CC(=Cc1ccc(C)cc1)[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	177.20
CAS:	52287-56-6

Physical Properties

Property code	Value	Unit	Source
gf	243.32	kJ/mol	Joback Method
hf	72.00	kJ/mol	Joback Method
hfus	25.56	kJ/mol	Joback Method
hvap	57.42	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.633		Crippen Method
mcvol	141.120	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	615.74	K	Joback Method
tc	865.48	K	Joback Method
tf	365.97	K	Joback Method
vc	0.550	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.75	J/mol×K	615.74	Joback Method
cpg	350.25	J/mol×K	657.36	Joback Method
cpg	362.72	J/mol×K	698.99	Joback Method
cpg	374.22	J/mol×K	740.61	Joback Method
cpg	384.84	J/mol×K	782.24	Joback Method
cpg	394.66	J/mol×K	823.86	Joback Method
cpg	403.75	J/mol×K	865.48	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=C52287566&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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