Benzene, 1-fluoro-4-(2-nitro-1-propenyl)-

Other names: Benzene, 1-fluoro-4-(2-nitropropenyl)-
p-Fluoro-«beta»-nitropropenylbenzene
Inchi: InChI=1S/C9H8FNO2/c1-7(11(12)13)6-8-2-4-9(10)5-3-8/h2-6H,1H3/b7-6+
InchiKey: VOAXWARMFBBINZ-VOTSOKGWSA-N
Formula: C9H8FNO2
SMILES: CC(=Cc1ccc(F)cc1)[N+](=O)[O-]
Mol. weight [g/mol]: 181.16
CAS: 775-31-5

Physical Properties

Property code	Value	Unit	Source
gf	40.09	kJ/mol	Joback Method
hf	-103.47	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	54.38	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.463		Crippen Method
mcvol	128.800	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	592.13	K	Joback Method
tc	834.59	K	Joback Method
tf	355.29	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.34	J/mol×K	592.13	Joback Method
cpg	310.30	J/mol×K	632.54	Joback Method
cpg	321.32	J/mol×K	672.95	Joback Method
cpg	331.48	J/mol×K	713.36	Joback Method
cpg	340.84	J/mol×K	753.77	Joback Method
cpg	349.46	J/mol×K	794.18	Joback Method
cpg	357.42	J/mol×K	834.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C775315&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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