3-(NO2)C6H4C(CH3)=CH2

Inchi: InChI=1S/C9H9NO2/c1-7(2)8-4-3-5-9(6-8)10(11)12/h3-6H,1H2,2H3
InchiKey: WMTKDRPCKOBHGI-UHFFFAOYSA-N
Formula: C9H9NO2
SMILES: C=C(C)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 163.17
CAS: 64416-49-5

Physical Properties

Property code	Value	Unit	Source
affp	812.20	kJ/mol	NIST Webbook
basg	783.30	kJ/mol	NIST Webbook
gf	242.52	kJ/mol	Joback Method
hf	100.85	kJ/mol	Joback Method
hfus	21.49	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.628		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	585.38	K	Joback Method
tc	835.06	K	Joback Method
tf	358.02	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.37	J/mol×K	585.38	Joback Method
cpg	302.95	J/mol×K	626.99	Joback Method
cpg	314.56	J/mol×K	668.61	Joback Method
cpg	325.27	J/mol×K	710.22	Joback Method
cpg	335.12	J/mol×K	751.83	Joback Method
cpg	344.19	J/mol×K	793.45	Joback Method
cpg	352.53	J/mol×K	835.06	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64416495&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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