3-NO2-C6H4CON(CH3)2

Inchi: InChI=1S/C9H10N2O3/c1-10(2)9(12)7-4-3-5-8(6-7)11(13)14/h3-6H,1-2H3
InchiKey: DKWDGIRXGDSOST-UHFFFAOYSA-N
Formula: C9H10N2O3
SMILES: CN(C)C(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 194.19
CAS: 7291-02-3

Physical Properties

Property code	Value	Unit	Source
affp	900.90	kJ/mol	NIST Webbook
basg	869.90	kJ/mol	NIST Webbook
gf	145.09	kJ/mol	Joback Method
hf	-59.84	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	63.95	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.297		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	655.13	K	Joback Method
tc	897.20	K	Joback Method
tf	456.14	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.35	J/mol×K	655.13	Joback Method
cpg	371.46	J/mol×K	695.48	Joback Method
cpg	382.60	J/mol×K	735.82	Joback Method
cpg	392.81	J/mol×K	776.17	Joback Method
cpg	402.17	J/mol×K	816.51	Joback Method
cpg	410.71	J/mol×K	856.86	Joback Method
cpg	418.50	J/mol×K	897.20	Joback Method

Sources

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=C7291023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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