1-(Nitromethyl)cyclopentene

Inchi: InChI=1S/C6H9NO2/c8-7(9)5-6-3-1-2-4-6/h3H,1-2,4-5H2
InchiKey: RURSHZDZIHCFLS-UHFFFAOYSA-N
Formula: C6H9NO2
SMILES: O=[N+]([O-])CC1=CCCC1
Mol. weight [g/mol]: 127.14
CAS: 2562-42-7

Physical Properties

Property code	Value	Unit	Source
gf	99.78	kJ/mol	Joback Method
hf	-50.80	kJ/mol	Joback Method
hfus	16.35	kJ/mol	Joback Method
hvap	47.06	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.373		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	512.61	K	Joback Method
tc	751.82	K	Joback Method
tf	329.41	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.45	J/mol×K	512.61	Joback Method
cpg	227.75	J/mol×K	552.48	Joback Method
cpg	239.18	J/mol×K	592.35	Joback Method
cpg	249.78	J/mol×K	632.22	Joback Method
cpg	259.61	J/mol×K	672.08	Joback Method
cpg	268.72	J/mol×K	711.95	Joback Method
cpg	277.15	J/mol×K	751.82	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=C2562427&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
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