Pentane, 2-nitro-

Inchi: InChI=1S/C5H11NO2/c1-3-4-5(2)6(7)8/h5H,3-4H2,1-2H3
InchiKey: JOIWPCUDRRYOQH-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: CCCC(C)[N+](=O)[O-]
Mol. weight [g/mol]: 117.15
CAS: 4609-89-6

Physical Properties

Property code	Value	Unit	Source
gf	24.33	kJ/mol	Joback Method
hf	-162.57	kJ/mol	Joback Method
hfus	16.54	kJ/mol	Joback Method
hvap	42.93	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.452		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	465.20	K	Joback Method
tc	674.41	K	Joback Method
tf	274.72	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.31	J/mol×K	465.20	Joback Method
cpg	220.22	J/mol×K	500.07	Joback Method
cpg	230.58	J/mol×K	534.94	Joback Method
cpg	240.40	J/mol×K	569.81	Joback Method
cpg	249.70	J/mol×K	604.68	Joback Method
cpg	258.50	J/mol×K	639.54	Joback Method
cpg	266.81	J/mol×K	674.41	Joback Method

Sources

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=C4609896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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