Pentane, 2,4-dimethyl-2-nitro-

Inchi: InChI=1S/C7H15NO2/c1-6(2)5-7(3,4)8(9)10/h6H,5H2,1-4H3
InchiKey: JOTFJIBCIJGTAS-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CC(C)CC(C)(C)[N+](=O)[O-]
Mol. weight [g/mol]: 145.20
CAS: 597-45-5

Physical Properties

Property code	Value	Unit	Source
gf	44.01	kJ/mol	Joback Method
hf	-212.60	kJ/mol	Joback Method
hfus	14.31	kJ/mol	Joback Method
hvap	46.08	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.088		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
tb	507.73	K	Joback Method
tc	724.36	K	Joback Method
tf	299.68	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.81	J/mol×K	507.73	Joback Method
cpg	311.02	J/mol×K	543.84	Joback Method
cpg	324.33	J/mol×K	579.94	Joback Method
cpg	336.79	J/mol×K	616.05	Joback Method
cpg	348.45	J/mol×K	652.15	Joback Method
cpg	359.35	J/mol×K	688.26	Joback Method
cpg	369.53	J/mol×K	724.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C597455&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