2-Nitro-1-pentanol

Inchi: InChI=1S/C5H11NO3/c1-2-3-5(4-7)6(8)9/h5,7H,2-4H2,1H3
InchiKey: OYHTVILGINELNJ-UHFFFAOYSA-N
Formula: C5H11NO3
SMILES: CCCC(CO)[N+](=O)[O-]
Mol. weight [g/mol]: 133.15
CAS: 2899-90-3

Physical Properties

Property code	Value	Unit	Source
gf	-112.49	kJ/mol	Joback Method
hf	-314.80	kJ/mol	Joback Method
hfus	20.63	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	0.424		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
ripol	2140.00		NIST Webbook
tb	557.38	K	Joback Method
tc	753.42	K	Joback Method
tf	335.54	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.45	J/mol×K	557.38	Joback Method
cpg	262.64	J/mol×K	590.05	Joback Method
cpg	271.35	J/mol×K	622.73	Joback Method
cpg	279.60	J/mol×K	655.40	Joback Method
cpg	287.41	J/mol×K	688.07	Joback Method
cpg	294.79	J/mol×K	720.75	Joback Method
cpg	301.75	J/mol×K	753.42	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=C2899903&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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