2-Nitro-2-methyl-1-butanol

Inchi: InChI=1S/C5H11NO3/c1-3-5(2,4-7)6(8)9/h7H,3-4H2,1-2H3
InchiKey: SEAMRWZKMYUKOI-UHFFFAOYSA-N
Formula: C5H11NO3
SMILES: CCC(C)(CO)[N+](=O)[O-]
Mol. weight [g/mol]: 133.15

Physical Properties

Property code	Value	Unit	Source
gf	-107.21	kJ/mol	Joback Method
hf	-318.27	kJ/mol	Joback Method
hfus	16.74	kJ/mol	Joback Method
hvap	58.70	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	0.424		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
ripol	2000.00		NIST Webbook
tb	554.59	K	Joback Method
tc	758.11	K	Joback Method
tf	352.96	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.85	J/mol×K	554.59	Joback Method
cpg	266.36	J/mol×K	588.51	Joback Method
cpg	275.26	J/mol×K	622.43	Joback Method
cpg	283.59	J/mol×K	656.35	Joback Method
cpg	291.38	J/mol×K	690.27	Joback Method
cpg	298.67	J/mol×K	724.19	Joback Method
cpg	305.49	J/mol×K	758.11	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=R307981&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