2-Nitro-3-methyl-1-butanol

Inchi: InChI=1S/C5H11NO3/c1-4(2)5(3-7)6(8)9/h4-5,7H,3H2,1-2H3
InchiKey: DMIRKUOHEBAINR-UHFFFAOYSA-N
Formula: C5H11NO3
SMILES: CC(C)C(CO)[N+](=O)[O-]
Mol. weight [g/mol]: 133.15
CAS: 77392-54-2

Physical Properties

Property code	Value	Unit	Source
gf	-114.93	kJ/mol	Joback Method
hf	-320.08	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	59.22	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	0.280		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
tb	556.94	K	Joback Method
tc	757.03	K	Joback Method
tf	320.54	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.86	J/mol×K	556.94	Joback Method
cpg	263.29	J/mol×K	590.29	Joback Method
cpg	272.23	J/mol×K	623.64	Joback Method
cpg	280.67	J/mol×K	656.98	Joback Method
cpg	288.65	J/mol×K	690.33	Joback Method
cpg	296.16	J/mol×K	723.68	Joback Method
cpg	303.25	J/mol×K	757.03	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=C77392542&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