2-Nitro-2-isopropyl-1,3-propanediol

Inchi: InChI=1S/C6H13NO4/c1-5(2)6(3-8,4-9)7(10)11/h5,8-9H,3-4H2,1-2H3
InchiKey: UREFUUVULNQGAM-UHFFFAOYSA-N
Formula: C6H13NO4
SMILES: CC(C)C(CO)(CO)[N+](=O)[O-]
Mol. weight [g/mol]: 163.17
CAS: 62155-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-238.05	kJ/mol	Joback Method
hf	-496.42	kJ/mol	Joback Method
hfus	19.90	kJ/mol	Joback Method
hvap	77.22	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	-0.357		Crippen Method
mcvol	124.560	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	669.21	K	Joback Method
tc	862.16	K	Joback Method
tf	410.05	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.53	J/mol×K	669.21	Joback Method
cpg	355.16	J/mol×K	701.37	Joback Method
cpg	363.26	J/mol×K	733.53	Joback Method
cpg	370.87	J/mol×K	765.68	Joback Method
cpg	378.01	J/mol×K	797.84	Joback Method
cpg	384.72	J/mol×K	830.00	Joback Method
cpg	391.04	J/mol×K	862.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62155311&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