iso-Propyl nitrite

Inchi: InChI=1S/C3H7NO2/c1-3(2)6-4-5/h3H,1-2H3
InchiKey: SKRDXYBATCVEMS-UHFFFAOYSA-N
Formula: C3H7NO2
SMILES: CC(C)ON=O
Mol. weight [g/mol]: 89.09
CAS: 541-42-4

Physical Properties

Property code	Value	Unit	Source
affp	845.50	kJ/mol	NIST Webbook
basg	813.00	kJ/mol	NIST Webbook
chl	-2017.00 ± 0.80	kJ/mol	NIST Webbook
hf	-133.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-164.00	kJ/mol	NIST Webbook
hvap	31.00	kJ/mol	NIST Webbook
ie	10.23 ± 0.01	eV	NIST Webbook
log10ws	-1.46		Crippen Method
logp	1.093		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	318.00	K	NIST Webbook
tb	313.10 ± 0.30	K	NIST Webbook
tb	313.30 ± 0.50	K	NIST Webbook
tc	526.38	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	26.00	kJ/mol	260.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541424&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

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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