

2-Bornanone, 3-nitro-, d-

Inchi:	InChI=1S/C10H15NO3/c1-9(2)6-4-5-10(9,3)8(12)7(6)11(13)14/h6-7H,4-5H2,1-3H3
InchiKey:	SYWPFHYANKVSU-UHFFFAOYSA-N
Formula:	C10H15NO3
SMILES:	CC12CCC(C([N+](=O)[O-])C1=O)C2(C)C
Mol. weight [g/mol]:	197.23
CAS:	2243-88-1

Physical Properties

Property code	Value	Unit	Source
gf	29.28	kJ/mol	Joback Method
hf	-268.95	kJ/mol	Joback Method
hfus	16.24	kJ/mol	Joback Method
hvap	55.77	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.657		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	656.75	K	Joback Method
tc	915.47	K	Joback Method
tf	485.97	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.92	J/molxK	656.75	Joback Method
cpg	450.99	J/molxK	699.87	Joback Method
cpg	467.36	J/molxK	742.99	Joback Method
cpg	483.40	J/molxK	786.11	Joback Method
cpg	499.44	J/molxK	829.23	Joback Method
cpg	515.84	J/molxK	872.35	Joback Method
cpg	532.94	J/molxK	915.47	Joback Method

Sources

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=C2243881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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