Tricyclo[3.3.1.13,7]decane, 2-nitro-

Other names: 2-Nitroadamantane
Inchi: InChI=1S/C10H15NO2/c12-11(13)10-8-2-6-1-7(4-8)5-9(10)3-6/h6-10H,1-5H2
InchiKey: ZFSCSQSQXFIKKH-UHFFFAOYSA-N
Formula: C10H15NO2
SMILES: O=[N+]([O-])C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 181.24

Physical Properties

Property code	Value	Unit	Source
chs	-5841.00 ± 2.20	kJ/mol	NIST Webbook
hf	-179.80 ± 3.20	kJ/mol	NIST Webbook
hfs	-237.80 ± 2.20	kJ/mol	NIST Webbook
hfus	27.46	kJ/mol	Joback Method
hsub	58.00 ± 2.30	kJ/mol	NIST Webbook
ie	9.83	eV	Cheméo Relay (1.0)
logp	2.088		Crippen Method
mcvol	136.600	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.47	J/mol×K	595.19	Joback Method
cpg	414.67	J/mol×K	635.83	Joback Method
cpg	432.36	J/mol×K	676.48	Joback Method
cpg	448.69	J/mol×K	717.12	Joback Method
cpg	463.79	J/mol×K	757.77	Joback Method
cpg	477.79	J/mol×K	798.41	Joback Method
cpg	490.84	J/mol×K	839.06	Joback Method
hfust	4.23	kJ/mol	452.20	NIST Webbook
hsubt	58.00 ± 2.30	kJ/mol	349.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54564317&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume