Tricyclo[3.3.1.1(3,7)]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]: 181.23
CAS: 54564-31-7

Physical Properties

Property code	Value	Unit	Source
chs	-5841.00 ± 2.20	kJ/mol	NIST Webbook
gf	223.60	kJ/mol	Joback Method
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
hvap	53.74	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.088		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	595.19	K	Joback Method
tc	839.06	K	Joback Method
tf	387.89	K	Joback Method
vc	0.538	m3/kmol	Joback 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
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=C54564317&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
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
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