Tricyclo[3.3.1.1(3,7)]decane, 1-nitro-

Other names: Adamantane, 1-nitro-
1-Nitroadamantane
Tricyclo[3.3.1.13,7]decane, 1-nitro-
Inchi: InChI=1S/C10H15NO2/c12-11(13)10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9H,1-6H2
InchiKey: HONLSNLUVRQMEK-UHFFFAOYSA-N
Formula: C10H15NO2
SMILES: O=[N+]([O-])C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 181.23
CAS: 7575-82-8

Physical Properties

Property code	Value	Unit	Source
chs	-5819.90 ± 2.20	kJ/mol	NIST Webbook
gf	225.82	kJ/mol	Joback Method
hf	-191.10 ± 2.40	kJ/mol	NIST Webbook
hfs	-254.70 ± 2.20	kJ/mol	NIST Webbook
hfus	20.09	kJ/mol	Joback Method
hsub	63.60 ± 1.00	kJ/mol	NIST Webbook
hvap	52.90	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.232		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	600.10	K	Joback Method
tc	854.16	K	Joback Method
tf	416.03	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.76	J/mol×K	600.10	Joback Method

cpg	410.07	J/mol×K	642.44	Joback Method
cpg	426.93	J/mol×K	684.79	Joback Method
cpg	442.62	J/mol×K	727.13	Joback Method
cpg	457.46	J/mol×K	769.47	Joback Method
cpg	471.75	J/mol×K	811.82	Joback Method
cpg	485.79	J/mol×K	854.16	Joback Method
hfust	4.18	kJ/mol	435.20	NIST Webbook
hsubt	63.60 ± 1.00	kJ/mol	339.00	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=C7575828&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume