

1-Adamantyl isocyanide

Inchi:	InChI=1S/C11H15N/c1-12-11-5-8-2-9(6-11)4-10(3-8)7-11/h8-10H,2-7H2
InchiKey:	RPRJRJNIFAYHRF-UHFFFAOYSA-N
Formula:	C11H15N
SMILES:	[C-]#[N+]C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	161.24
CAS:	22110-53-8

Physical Properties

Property code	Value	Unit	Source
chs	-6464.10 ± 1.90	kJ/mol	NIST Webbook
gf	331.87	kJ/mol	Joback Method
hf	73.10 ± 2.00	kJ/mol	NIST Webbook
hfs	-8.30 ± 1.90	kJ/mol	NIST Webbook
hfus	12.83	kJ/mol	Joback Method
hsub	81.42 ± 0.46	kJ/mol	NIST Webbook
hsub	81.40	kJ/mol	NIST Webbook
hvap	49.01	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	2.874		Crippen Method
mcvol	134.650	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	573.22	K	Joback Method
tc	811.33	K	Joback Method
tf	348.68	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.36	J/mol×K	573.22	Joback Method
cpg	382.83	J/mol×K	612.91	Joback Method
cpg	398.92	J/mol×K	652.59	Joback Method
cpg	413.87	J/mol×K	692.28	Joback Method
cpg	427.94	J/mol×K	731.96	Joback Method

cpg	441.36	J/mol×K	771.65	Joback Method
cpg	454.38	J/mol×K	811.33	Joback Method
cps	215.20	J/mol×K	298.15	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22110538&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hsub:	Enthalpy of sublimation 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

Latest version available from:

<https://www.chemeo.com/cid/16-195-8/1-Adamantyl-isocyanide.pdf>

Generated by Cheméo on 2025-12-05 21:54:43.690969379 +0000 UTC m=+4719881.221010045.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.