1-Adamantanecarboxamide, N,N-dimethyl-

Other names: Tricyclo[3.3.1.13,7]decane-1-carboxamide, N,N-dimethyl-
N,N-Dimethyl-1-adamantanecarboxamide
N,N-Dimethyl-1-adamantylcarboxamide
Inchi: InChI=1S/C13H21NO/c1-14(2)12(15)13-6-9-3-10(7-13)5-11(4-9)8-13/h9-11H,3-8H2,1-2H
InchiKey: RMRZPLJAVNSFCJ-UHFFFAOYSA-N
Formula: C13H21NO
SMILES: CN(C)C(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 207.31
CAS: 1502-00-7

Physical Properties

Property code	Value	Unit	Source
affp	949.40	kJ/mol	NIST Webbook
basg	917.60	kJ/mol	NIST Webbook
chs	-7733.20 ± 2.10	kJ/mol	NIST Webbook
gf	197.39	kJ/mol	Joback Method
hf	-286.10 ± 2.70	kJ/mol	NIST Webbook
hfs	-383.60 ± 2.70	kJ/mol	NIST Webbook
hfus	21.12	kJ/mol	Joback Method
hsub	97.50 ± 0.30	kJ/mol	NIST Webbook
hsub	97.50 ± 0.30	kJ/mol	NIST Webbook
hvap	51.77	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.291		Crippen Method
mcvol	173.000	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	583.21	K	Joback Method
tc	801.50	K	Joback Method
tf	388.63	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	575.07	J/mol×K	765.12	Joback Method
cpg	484.64	J/mol×K	583.21	Joback Method
cpg	505.23	J/mol×K	619.59	Joback Method
cpg	524.36	J/mol×K	655.97	Joback Method
cpg	542.24	J/mol×K	692.36	Joback Method
cpg	559.08	J/mol×K	728.74	Joback Method
cpg	590.44	J/mol×K	801.50	Joback Method
hsubt	96.90 ± 0.30	kJ/mol	312.50	NIST Webbook

Sources

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=C1502007&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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