

N,N-DIMETHYL-1-ADAMANTANECARBOXAMIDE

Other names:	Tricyclo[3.3.1.1 ^{3,7}]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,3-8H2,1-2H3
InchiKey:	RMRZPLJAVNSFCJ-UHFFFAOYSA-N
Formula:	C13H21NO
SMILES:	CN(C)C(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	207.32

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
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
ie	8.50	eV	Cheméo Relay (1.0)
logp	2.291		Crippen Method
mcvol	173.000	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	575.07	J/mol×K	765.12	Joback Method
cpg	590.44	J/mol×K	801.50	Joback Method
hsubt	96.90 ± 0.30	kJ/mol	312.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1502007&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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

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