

N-(Adamantan-1-yl)formamide

Other names:	N-(1-Adamantyl)formamide
Inchi:	InChI=1S/C11H17NO/c13-7-12-11-4-8-1-9(5-11)3-10(2-8)6-11/h7-10H,1-6H2,(H,12,13)
InchiKey:	BUPHJFOIWZKPNV-BIBSGERRSA-N
Formula:	C11H17NO
SMILES:	O=CNC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	179.26

Physical Properties

Property code	Value	Unit	Source
hfus	18.71	kJ/mol	Joback Method
logp	1.701		Crippen Method
mcpvol	144.820	ml/mol	McGowan Method
rinpol	1693.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.25	J/mol×K	569.97	Joback Method
cpg	420.53	J/mol×K	607.28	Joback Method
cpg	437.44	J/mol×K	644.58	Joback Method
cpg	453.18	J/mol×K	681.89	Joback Method
cpg	467.96	J/mol×K	719.19	Joback Method
cpg	481.98	J/mol×K	756.50	Joback Method
cpg	495.46	J/mol×K	793.81	Joback Method

Sources

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):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3405489&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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