Formamide, N-(1-adamantyl)-

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)/t
InchiKey: BUPHJFOIWZKPNV-BIBSGERRSA-N
Formula: C11H17NO
SMILES: O=CNC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 179.26
CAS: 3405-48-9

Physical Properties

Property code	Value	Unit	Source
gf	188.56	kJ/mol	Joback Method
hf	-95.34	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	51.69	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.701		Crippen Method
mcvol	144.820	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1693.00		NIST Webbook
tb	569.97	K	Joback Method
tc	793.81	K	Joback Method
tf	378.35	K	Joback Method
vc	0.564	m3/kmol	Joback Method

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

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=C3405489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume