Formamide, N-(2-adamantyl)

Inchi: InChI=1S/C11H17NO/c13-6-12-11-9-2-7-1-8(4-9)5-10(11)3-7/h6-11H,1-5H2,(H,12,13)
InchiKey: SXYGFWZEAKCCIZ-UHFFFAOYSA-N
Formula: C11H17NO
SMILES: O=CNC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 179.26

Physical Properties

Property code	Value	Unit	Source
gf	186.34	kJ/mol	Joback Method
hf	-130.92	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	52.53	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.557		Crippen Method
mcvol	144.820	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	565.06	K	Joback Method
tc	780.11	K	Joback Method
tf	350.21	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.63	J/mol×K	565.06	Joback Method
cpg	423.65	J/mol×K	600.90	Joback Method
cpg	441.37	J/mol×K	636.74	Joback Method
cpg	457.88	J/mol×K	672.59	Joback Method
cpg	473.27	J/mol×K	708.43	Joback Method
cpg	487.64	J/mol×K	744.27	Joback Method
cpg	501.08	J/mol×K	780.11	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=R44469&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