Adamantan-4-one, 1-amino

Inchi: InChI=1S/C10H15NO/c11-10-3-6-1-7(4-10)9(12)8(2-6)5-10/h6-8H,1-5,11H2
InchiKey: FXBKMQRDMLOJNV-UHFFFAOYSA-N
Formula: C10H15NO
SMILES: NC12CC3CC(C1)C(=O)C(C3)C2
Mol. weight [g/mol]: 165.23

Physical Properties

Property code	Value	Unit	Source
gf	134.13	kJ/mol	Joback Method
hf	-146.50	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	51.19	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.093		Crippen Method
mcvol	130.730	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	588.61	K	Joback Method
tc	838.61	K	Joback Method
tf	423.90	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.64	J/mol×K	588.61	Joback Method
cpg	393.05	J/mol×K	630.28	Joback Method
cpg	410.14	J/mol×K	671.94	Joback Method
cpg	426.13	J/mol×K	713.61	Joback Method
cpg	441.27	J/mol×K	755.28	Joback Method
cpg	455.78	J/mol×K	796.95	Joback Method
cpg	469.90	J/mol×K	838.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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