Adamantylurea

Inchi: InChI=1S/C11H18N2O/c12-10(14)13-11-4-7-1-8(5-11)3-9(2-7)6-11/h7-9H,1-6H2,(H3,12,
InchiKey: QYYHPAUOLCHORH-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: NC(=O)NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	225.61	kJ/mol	Joback Method
hf	-88.55	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	62.35	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.623		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1302.00		NIST Webbook
tb	647.71	K	Joback Method
tc	883.93	K	Joback Method
tf	469.54	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.53	J/mol×K	647.71	Joback Method
cpg	484.90	J/mol×K	687.08	Joback Method
cpg	501.16	J/mol×K	726.45	Joback Method
cpg	516.56	J/mol×K	765.82	Joback Method
cpg	531.34	J/mol×K	805.19	Joback Method
cpg	545.74	J/mol×K	844.56	Joback Method
cpg	560.01	J/mol×K	883.93	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=R231384&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