Adamantane-2-carboxylic acid

Inchi: InChI=1S/C11H16O2/c12-11(13)10-8-2-6-1-7(4-8)5-9(10)3-6/h6-10H,1-5H2,(H,12,13)
InchiKey: UNGMXQVELCJRIH-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: O=C(O)C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 180.24
CAS: 15897-81-1

Physical Properties

Property code	Value	Unit	Source
chs	-5988.10 ± 3.80	kJ/mol	NIST Webbook
gf	-69.27	kJ/mol	Joback Method
hf	-363.62	kJ/mol	Joback Method
hfs	-627.18	kJ/mol	NIST Webbook
hfus	24.38	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.143		Crippen Method
mcvol	140.710	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	612.28	K	Joback Method
tc	816.90	K	Joback Method
tf	366.30	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.96	J/mol×K	612.28	Joback Method
cpg	429.92	J/mol×K	646.38	Joback Method
cpg	444.84	J/mol×K	680.49	Joback Method
cpg	458.81	J/mol×K	714.59	Joback Method
cpg	471.89	J/mol×K	748.69	Joback Method
cpg	484.18	J/mol×K	782.80	Joback Method
cpg	495.74	J/mol×K	816.90	Joback Method

dvisc	0.0060810	Pa×s	366.30	Joback Method
dvisc	0.0040463	Pa×s	407.30	Joback Method
dvisc	0.0029007	Pa×s	448.29	Joback Method
dvisc	0.0021987	Pa×s	489.29	Joback Method
dvisc	0.0017396	Pa×s	530.29	Joback Method
dvisc	0.0014234	Pa×s	571.28	Joback Method
dvisc	0.0011964	Pa×s	612.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15897811&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.