

Adamantane-1-carboxylic acid

Other names:	1-adamantanecarboxylic acid Tricyclo[3.3.1.1 tricyclo[3.3.1.1(3,7)]decane-1-carboxylic acid
Inchi:	InChI=1S/C11H16O2/c12-10(13)11-4-7-1-8(5-11)3-9(2-7)6-11/h7-9H,1-6H2,(H,12,13)
InchiKey:	JIMXXGFJRDUSRO-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	O=C(O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	180.24
CAS:	828-51-3

Physical Properties

Property code	Value	Unit	Source
chs	-5972.20 ± 3.60	kJ/mol	NIST Webbook
gf	-67.05	kJ/mol	Joback Method
hf	-328.04	kJ/mol	Joback Method
hfs	-643.08	kJ/mol	NIST Webbook
hfus	16.20	kJ/mol	The Joining of Measurement and Prediction: The Enthalpy of Formation of 1,4-Cubanedicarboxylic Acid
hvap	61.96	kJ/mol	Joback Method
ie	9.34	eV	NIST Webbook
log10ws	-2.24		Crippen Method
logp	2.287		Crippen Method
mcvol	140.710	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
rinpol	1433.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2118.00		NIST Webbook
tb	617.19	K	Joback Method
tc	829.42	K	Joback Method
tf	394.44	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.20	J/mol×K	758.68	Joback Method
cpg	477.54	J/mol×K	794.05	Joback Method
cpg	409.61	J/mol×K	617.19	Joback Method
cpg	424.80	J/mol×K	652.56	Joback Method
cpg	439.00	J/mol×K	687.93	Joback Method
cpg	452.41	J/mol×K	723.31	Joback Method
cpg	489.60	J/mol×K	829.42	Joback Method
hfust	2.25	kJ/mol	524.20	NIST Webbook
hfust	2.25	kJ/mol	524.20	NIST Webbook

Sources

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=C828513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Joining of Measurement and Prediction: The Enthalpy of Formation of 1,4-Cubanedicarboxylic Acid:	https://www.doi.org/10.1021/je101124p

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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