

1-Adamantaneacetic acid

Other names:	Tricyclo[3.3.1.1(3,7)-]decane-1-acetic acid 1-Adamantylacetic acid tricyclo[3.3.1.13,7]dec-1-ylacetic acid
Inchi:	InChI=1S/C12H18O2/c13-11(14)7-12-4-8-1-9(5-12)3-10(2-8)6-12/h8-10H,1-7H2,(H,13,14)
InchiKey:	AOTQGWFNFTVXNQ-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	O=C(O)CC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	194.27
CAS:	4942-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-58.63	kJ/mol	Joback Method
hf	-348.68	kJ/mol	Joback Method
hfus	19.60	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.678		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	640.07	K	Joback Method
tc	848.95	K	Joback Method
tf	405.71	K	Joback Method
vc	0.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.29	J/mol×K	640.07	Joback Method
cpg	475.95	J/mol×K	674.88	Joback Method
cpg	490.70	J/mol×K	709.70	Joback Method
cpg	504.72	J/mol×K	744.51	Joback Method
cpg	518.16	J/mol×K	779.32	Joback Method
cpg	531.21	J/mol×K	814.14	Joback Method

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=C4942476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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