Adamantan-2-ol

Other names: Tricyclo[3.3.1.1
Inchi: InChI=1S/C10H16O/c11-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-11H,1-5H2
InchiKey: FOWDOWQYRZXQDP-UHFFFAOYSA-N
Formula: C10H16O
SMILES: OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 152.23
CAS: 700-57-2

Physical Properties

Property code	Value	Unit	Source
chs	-5834.00 ± 4.00	kJ/mol	NIST Webbook
gf	51.23	kJ/mol	Joback Method
hf	-299.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-388.00 ± 4.00	kJ/mol	NIST Webbook
hfus	20.19	kJ/mol	Joback Method
hsub	88.10 ± 1.60	kJ/mol	NIST Webbook
hsub	89.00 ± 3.00	kJ/mol	NIST Webbook
hsub	89.00	kJ/mol	NIST Webbook
hsub	88.70 ± 2.50	kJ/mol	NIST Webbook
hvap	53.83	kJ/mol	Joback Method
ie	9.09 ± 0.07	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
log10ws	-2.10		Crippen Method
logp	1.803		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1405.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1358.00		NIST Webbook

ripol	1944.00		NIST Webbook
ripol	1944.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	1962.00		NIST Webbook
tb	535.53	K	Joback Method
tc	735.26	K	Joback Method
tf	305.10	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.51	J/mol×K	602.11	Joback Method
cpg	429.29	J/mol×K	735.26	Joback Method
cpg	416.86	J/mol×K	701.97	Joback Method
cpg	403.64	J/mol×K	668.68	Joback Method
cpg	389.55	J/mol×K	635.39	Joback Method
cpg	341.31	J/mol×K	535.53	Joback Method
cpg	358.46	J/mol×K	568.82	Joback Method
dvisc	0.0035397	Pa×s	343.50	Joback Method
dvisc	0.0025337	Pa×s	381.91	Joback Method
dvisc	0.0019279	Pa×s	420.31	Joback Method
dvisc	0.0015356	Pa×s	458.72	Joback Method
dvisc	0.0012669	Pa×s	497.12	Joback Method
dvisc	0.0053793	Pa×s	305.10	Joback Method
dvisc	0.0010745	Pa×s	535.53	Joback Method
hfust	3.74	kJ/mol	391.20	NIST Webbook
hfust	0.30	kJ/mol	325.20	NIST Webbook
hfust	11.94	kJ/mol	567.30	NIST Webbook
sfust	9.56	J/mol×K	391.20	NIST Webbook
sfust	0.92	J/mol×K	325.20	NIST Webbook

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

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume