Diamantan-1-ol

Other names:	1-diamantanol
	1-hydroxydiamantane
	3,5,1,7-[1,2,3,4]butanetetraylnaphthalen-1(2H)-ol, octahydro-
Inchi:	InChI=1S/C14H20O/c15-14-6-8-2-10-9-1-7(4-12(10)14)5-13(14)11(9)3-8/h7-13,15H,1-6H
InchiKey:	ZTONXKOBHDGNKB-UHFFFAOYSA-N
Formula:	C14H20O
SMILES:	OC12CC3CC4C5CC(CC41)CC2C5C3
Mol. weight [g/mol]:	204.31
CAS:	30545-14-3

Physical Properties

Property code	Value	Unit	Source
chs	-7938.60 ± 1.00	kJ/mol	NIST Webbook
gf	217.41	kJ/mol	Joback Method
hf	-310.90 ± 1.20	kJ/mol	NIST Webbook
hfs	-428.80 ± 1.00	kJ/mol	NIST Webbook
hfus	25.79	kJ/mol	Joback Method
hsub	117.90	kJ/mol	NIST Webbook
hvap	60.75	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.440		Crippen Method
mcvol	159.690	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	627.56	K	Joback Method
tc	836.94	K	Joback Method
tf	412.76	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.21	J/mol×K	767.15	Joback Method
cpg	596.39	J/mol×K	802.04	Joback Method
cpg	513.33	J/mol×K	627.56	Joback Method

cpg	531.83	J/mol×K	662.46	Joback Method
cpg	549.16	J/mol×K	697.35	Joback Method
cpg	565.54	J/mol×K	732.25	Joback Method
cpg	611.31	J/mol×K	836.94	Joback Method
hfust	9.60	kJ/mol	573.00	NIST Webbook
hsubt	118.00 ± 0.60	kJ/mol	334.00	NIST Webbook
hsubt	117.90 ± 0.59	kJ/mol	334.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Diamantane, Trimantane, Tetramantane, and Their Derivatives in Organic Solvents:	https://www.doi.org/10.1021/je800277a
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=C30545143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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