Diamantan-3-ol

Inchi: InChI=1S/C14H20O/c15-14-7-4-9-8-1-6-2-11(9)13(14)12(3-6)10(8)5-7/h6-15H,1-5H2
InchiKey: WXZXBNQJFLBGEB-UHFFFAOYSA-N
Formula: C14H20O
SMILES: OC1C2CC3C4CC5CC3C1C(C5)C4C2
Mol. weight [g/mol]: 204.31
CAS: 30545-24-5

Physical Properties

Property code	Value	Unit	Source
chs	-7953.70 ± 1.50	kJ/mol	NIST Webbook
gf	215.19	kJ/mol	Joback Method
hf	-297.60 ± 4.60	kJ/mol	NIST Webbook
hfs	-413.80 ± 1.50	kJ/mol	NIST Webbook
hfus	33.16	kJ/mol	Joback Method
hsub	116.20	kJ/mol	NIST Webbook
hsub	116.10 ± 4.40	kJ/mol	NIST Webbook
hvap	61.59	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.295		Crippen Method
mcvol	159.690	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
tb	622.65	K	Joback Method
tc	824.70	K	Joback Method
tf	384.62	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.52	J/mol×K	622.65	Joback Method
cpg	536.70	J/mol×K	656.32	Joback Method
cpg	554.62	J/mol×K	690.00	Joback Method
cpg	571.42	J/mol×K	723.67	Joback Method
cpg	587.22	J/mol×K	757.35	Joback Method

cpg	602.17	J/mol×K	791.02	Joback Method
cpg	616.39	J/mol×K	824.70	Joback Method
dvisc	0.0082175	Pa×s	384.62	Joback Method
dvisc	0.0091342	Pa×s	424.29	Joback Method
dvisc	0.0099712	Pa×s	463.96	Joback Method
dvisc	0.0107356	Pa×s	503.63	Joback Method
dvisc	0.0114346	Pa×s	543.31	Joback Method
dvisc	0.0120750	Pa×s	582.98	Joback Method
dvisc	0.0126630	Pa×s	622.65	Joback Method
hsubt	116.10 ± 4.40	kJ/mol	338.50	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=C30545245&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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