2-isobutyl-2-adamantanol

Inchi: InChI=1S/C14H24O/c1-9(2)8-14(15)12-4-10-3-11(6-12)7-13(14)5-10/h9-13,15H,3-8H2,1-
InchiKey: ALXGUIIGZLCLNY-UHFFFAOYSA-N
Formula: C14H24O
SMILES: CC(C)CC1(O)C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	76.98	kJ/mol	Joback Method
hf	-303.00	kJ/mol	Joback Method
hfus	20.73	kJ/mol	Joback Method
hvap	61.19	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.220		Crippen Method
mcvol	181.410	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2061.00		NIST Webbook
tb	626.85	K	Joback Method
tc	826.66	K	Joback Method
tf	359.08	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.34	J/mol×K	626.85	Joback Method
cpg	563.24	J/mol×K	660.15	Joback Method

cpg	581.09	J/mol×K	693.45	Joback Method
cpg	598.04	J/mol×K	726.76	Joback Method
cpg	614.25	J/mol×K	760.06	Joback Method
cpg	629.86	J/mol×K	793.36	Joback Method
cpg	645.01	J/mol×K	826.66	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=R304566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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