2-propyl-2-adamantanol

Inchi: InChI=1S/C13H22O/c1-2-3-13(14)11-5-9-4-10(7-11)8-12(13)6-9/h9-12,14H,2-8H2,1H3
InchiKey: SEFJJPZJVPVBQK-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CCCC1(O)C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	71.00	kJ/mol	Joback Method
hf	-277.08	kJ/mol	Joback Method
hfus	21.66	kJ/mol	Joback Method
hvap	59.35	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.974		Crippen Method
mcvol	167.320	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2036.00		NIST Webbook
tb	604.41	K	Joback Method
tc	803.16	K	Joback Method
tf	362.81	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.06	J/mol×K	604.41	Joback Method
cpg	509.24	J/mol×K	637.53	Joback Method

cpg	526.35	J/mol×K	670.66	Joback Method
cpg	542.56	J/mol×K	703.78	Joback Method
cpg	557.99	J/mol×K	736.91	Joback Method
cpg	572.81	J/mol×K	770.03	Joback Method
cpg	587.14	J/mol×K	803.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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