

2-butyl-2-adamantanol

Inchi:	InChI=1S/C14H24O/c1-2-3-4-14(15)12-6-10-5-11(8-12)9-13(14)7-10/h10-13,15H,2-9H2,
InchiKey:	PXRAOOXXPGRCJZ-UHFFFAOYSA-N
Formula:	C14H24O
SMILES:	CCCCC1(O)C2CC3CC(C2)CC1C3
Mol. weight [g/mol]:	208.34

Physical Properties

Property code	Value	Unit	Source
gf	79.42	kJ/mol	Joback Method
hf	-297.72	kJ/mol	Joback Method
hfus	24.25	kJ/mol	Joback Method
hvap	61.58	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.364		Crippen Method
mcvol	181.410	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1637.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2143.00		NIST Webbook
tb	627.29	K	Joback Method
tc	823.46	K	Joback Method
tf	374.08	K	Joback Method
vc	0.698	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.95	J/molxK	627.29	Joback Method
cpg	562.46	J/molxK	659.99	Joback Method
cpg	579.97	J/molxK	692.68	Joback Method

cpg	596.62	J/mol×K	725.38	Joback Method
cpg	612.55	J/mol×K	758.07	Joback Method
cpg	627.91	J/mol×K	790.77	Joback Method
cpg	642.83	J/mol×K	823.46	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=R304526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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