

2-[1-Adamantyl]propan-2-ol

Other names:	2-(1-adamantyl)-2-propanol
Inchi:	InChI=1S/C13H22O/c1-12(2,14)13-6-9-3-10(7-13)5-11(4-9)8-13/h9-11,14H,3-8H2,1-2H3
InchiKey:	WBKAUEBLTWRERU-UHFFFAOYSA-N
Formula:	C13H22O
SMILES:	CC(C)(O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	194.31
CAS:	775-64-4

Physical Properties

Property code	Value	Unit	Source
gf	81.55	kJ/mol	Joback Method
hf	-265.49	kJ/mol	Joback Method
hfus	13.18	kJ/mol	Joback Method
hvap	58.37	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.974		Crippen Method
mcvol	167.320	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1550.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2059.00		NIST Webbook
tb	605.85	K	Joback Method
tc	816.02	K	Joback Method
tf	369.47	K	Joback Method
vc	0.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	492.61	J/mol×K	605.85	Joback Method
cpg	511.25	J/mol×K	640.88	Joback Method
cpg	528.63	J/mol×K	675.91	Joback Method
cpg	544.96	J/mol×K	710.94	Joback Method
cpg	560.44	J/mol×K	745.97	Joback Method
cpg	575.25	J/mol×K	781.00	Joback Method
cpg	589.60	J/mol×K	816.02	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=C775644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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