3-n-Propyl-adamantol-1

Other names: 3-propyl-1-adamantanol
Inchi: InChI=1S/C13H22O/c1-2-3-12-5-10-4-11(6-12)8-13(14,7-10)9-12/h10-11,14H,2-9H2,1H3
InchiKey: DASJOTIHKLXABK-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CCCC12CC3CC(CC(O)(C3)C1)C2
Mol. weight [g/mol]: 194.31
CAS: 15598-88-6

Physical Properties

Property code	Value	Unit	Source
gf	73.22	kJ/mol	Joback Method
hf	-241.50	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	58.51	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.118		Crippen Method
mcvol	167.320	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1495.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
tb	609.32	K	Joback Method
tc	815.40	K	Joback Method
tf	390.95	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.39	J/mol×K	609.32	Joback Method
cpg	504.87	J/mol×K	643.67	Joback Method
cpg	521.34	J/mol×K	678.01	Joback Method
cpg	537.04	J/mol×K	712.36	Joback Method
cpg	552.21	J/mol×K	746.70	Joback Method
cpg	567.10	J/mol×K	781.05	Joback Method
cpg	581.94	J/mol×K	815.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15598886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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