3-ethyl-1-adamantanol

Inchi: InChI=1S/C12H20O/c1-2-11-4-9-3-10(5-11)7-12(13,6-9)8-11/h9-10,13H,2-8H2,1H3
InchiKey: LJFGNNHKXSJWFF-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CCC12CC3CC(CC(O)(C3)C1)C2
Mol. weight [g/mol]: 180.29

Physical Properties

Property code	Value	Unit	Source
gf	64.80	kJ/mol	Joback Method
hf	-220.86	kJ/mol	Joback Method
hfus	11.70	kJ/mol	Joback Method
hvap	56.28	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.728		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1408.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1408.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	1969.00		NIST Webbook
tb	586.44	K	Joback Method
tc	795.77	K	Joback Method
tf	379.68	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.57	J/mol×K	586.44	Joback Method
cpg	453.66	J/mol×K	621.33	Joback Method

cpg	469.62	J/mol×K	656.22	Joback Method
cpg	484.71	J/mol×K	691.11	Joback Method
cpg	499.17	J/mol×K	726.00	Joback Method
cpg	513.26	J/mol×K	760.88	Joback Method
cpg	527.21	J/mol×K	795.77	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304704&Units=SI

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