3-butyl-1-adamantanol

Inchi: InChI=1S/C14H24O/c1-2-3-4-13-6-11-5-12(7-13)9-14(15,8-11)10-13/h11-12,15H,2-10H2
InchiKey: GSFQHLMKIMLFLH-UHFFFAOYSA-N
Formula: C14H24O
SMILES: CCCCC12CC3CC(CC(O)(C3)C1)C2
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	81.64	kJ/mol	Joback Method
hf	-262.14	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.508		Crippen Method
mcvol	181.410	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1641.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	632.20	K	Joback Method
tc	835.27	K	Joback Method
tf	402.22	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.57	J/mol×K	632.20	Joback Method
cpg	557.45	J/mol×K	666.05	Joback Method
cpg	574.43	J/mol×K	699.89	Joback Method
cpg	590.74	J/mol×K	733.74	Joback Method

cpg	606.62	J/mol×K	767.58	Joback Method
cpg	622.30	J/mol×K	801.43	Joback Method
cpg	638.02	J/mol×K	835.27	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=R304695&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

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