

1-Adamantaneethanol

Other names:	Tricyclo[3.3.1.1(3,7)-]decane-1-ethanol 2-(tricyclo(3.3.1.1'3,7)dec-1-yl)ethanol
Inchi:	InChI=1S/C12H20O/c13-2-1-12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11,13H,1-8H2
InchiKey:	ZBIDZPHRNBZTLT-UHFFFAOYSA-N
Formula:	C12H20O
SMILES:	OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	180.29
CAS:	6240-11-5

Physical Properties

Property code	Value	Unit	Source
gf	70.29	kJ/mol	Joback Method
hf	-236.10	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	57.44	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.585		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
tb	586.20	K	Joback Method
tc	787.89	K	Joback Method
tf	355.78	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.31	J/mol×K	586.20	Joback Method
cpg	455.65	J/mol×K	619.81	Joback Method
cpg	471.89	J/mol×K	653.43	Joback Method
cpg	487.18	J/mol×K	687.04	Joback Method
cpg	501.68	J/mol×K	720.66	Joback Method
cpg	515.54	J/mol×K	754.27	Joback Method
cpg	528.92	J/mol×K	787.89	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=C6240115&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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