

2-Norbornanethiol, acetate

Inchi:	InChI=1S/C9H14OS/c1-6(10)11-9-5-7-2-3-8(9)4-7/h7-9H,2-5H2,1H3
InchiKey:	AKEZPHRQPYDGQV-UHFFFAOYSA-N
Formula:	C9H14OS
SMILES:	CC(=O)SC1CC2CCC1C2
Mol. weight [g/mol]:	170.27
CAS:	90611-37-3

Physical Properties

Property code	Value	Unit	Source
gf	30.79	kJ/mol	Joback Method
hf	-180.70	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	48.88	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.455		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	541.05	K	Joback Method
tc	773.03	K	Joback Method
tf	303.64	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.64	J/molxK	541.05	Joback Method
cpg	342.79	J/molxK	579.71	Joback Method
cpg	358.76	J/molxK	618.38	Joback Method
cpg	373.60	J/molxK	657.04	Joback Method
cpg	387.39	J/molxK	695.70	Joback Method
cpg	400.20	J/molxK	734.36	Joback Method
cpg	412.09	J/molxK	773.03	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=C90611373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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