7,7-Dimethyl bicyclo [4.1.0] Heptan-3-ol

Inchi: InChI=1S/C9H16O/c1-9(2)7-4-3-6(10)5-8(7)9/h6-8,10H,3-5H2,1-2H3
InchiKey: PQKVVIGNGCACJY-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC1(C)C2CCC(O)CC21
Mol. weight [g/mol]: 140.22

Physical Properties

Property code	Value	Unit	Source
gf	-23.43	kJ/mol	Joback Method
hf	-267.32	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	50.54	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.803		Crippen Method
mcvol	121.820	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook
tb	506.15	K	Joback Method
tc	701.94	K	Joback Method
tf	299.79	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.80	J/mol×K	506.15	Joback Method
cpg	323.32	J/mol×K	538.78	Joback Method
cpg	337.82	J/mol×K	571.41	Joback Method
cpg	351.42	J/mol×K	604.04	Joback Method
cpg	364.21	J/mol×K	636.67	Joback Method
cpg	376.31	J/mol×K	669.30	Joback Method
cpg	387.81	J/mol×K	701.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R332051&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume