9-Aza-1-methylbicyclo[3.3.1]nonan-3-ol

Inchi: InChI=1S/C9H17NO/c1-9-4-2-3-7(10-9)5-8(11)6-9/h7-8,10-11H,2-6H2,1H3
InchiKey: DPTCGYGOXXZERV-UHFFFAOYSA-N
Formula: C9H17NO
SMILES: CC12CCCC(CC(O)C1)N2
Mol. weight [g/mol]: 155.24
CAS: 2038-40-6

Physical Properties

Property code	Value	Unit	Source
gf	47.79	kJ/mol	Joback Method
hf	-221.49	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	57.95	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.042		Crippen Method
mcvol	131.800	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	567.91	K	Joback Method
tc	783.13	K	Joback Method
tf	342.50 ± 0.50	K	NIST Webbook
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.37	J/mol×K	567.91	Joback Method
cpg	369.89	J/mol×K	603.78	Joback Method
cpg	385.38	J/mol×K	639.65	Joback Method
cpg	399.98	J/mol×K	675.52	Joback Method
cpg	413.82	J/mol×K	711.39	Joback Method
cpg	427.00	J/mol×K	747.26	Joback Method
cpg	439.67	J/mol×K	783.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.50 ± 2.50	K	0.01	NIST Webbook

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=C2038406&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume