3-Oxabicyclo[3,2,2]nonane

Inchi: InChI=1S/C8H14O/c1-2-8-4-3-7(1)5-9-6-8/h7-8H,1-6H2
InchiKey: SVSOGVQZYJCDKO-UHFFFAOYSA-N
Formula: C8H14O
SMILES: C1CC2CCC1COC2
Mol. weight [g/mol]: 126.20
CAS: 283-27-2

Physical Properties

Property code	Value	Unit	Source
chs	-4873.27 ± 0.88	kJ/mol	NIST Webbook
gf	15.56	kJ/mol	Joback Method
hf	-222.60 ± 1.00	kJ/mol	NIST Webbook
hfs	-275.70 ± 0.84	kJ/mol	NIST Webbook
hfus	14.42	kJ/mol	Joback Method
hsub	53.10	kJ/mol	NIST Webbook
hvap	38.25	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.823		Crippen Method
mcvol	107.730	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
sl	236.27	J/mol×K	NIST Webbook
tb	435.68	K	Joback Method
tc	654.15	K	Joback Method
tf	231.81	K	Joback Method
tt	448.43 ± 0.02	K	NIST Webbook
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.10	J/mol×K	435.68	Joback Method
cpg	248.80	J/mol×K	472.09	Joback Method
cpg	266.33	J/mol×K	508.50	Joback Method
cpg	282.76	J/mol×K	544.91	Joback Method

cpg	298.13	J/mol×K	581.32	Joback Method
cpg	312.50	J/mol×K	617.73	Joback Method
cpg	325.93	J/mol×K	654.15	Joback Method
cpl	185.06	J/mol×K	298.15	NIST Webbook
dvisc	0.0032638	Pa×s	231.81	Joback Method
dvisc	0.0019879	Pa×s	265.79	Joback Method
dvisc	0.0013548	Pa×s	299.77	Joback Method
dvisc	0.0009983	Pa×s	333.75	Joback Method
dvisc	0.0007784	Pa×s	367.72	Joback Method
dvisc	0.0006330	Pa×s	401.70	Joback Method
dvisc	0.0005316	Pa×s	435.68	Joback Method
hfust	6.75	kJ/mol	448.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C283272&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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

sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume