3-oxatricyclo[3.2.1.02,4]octane

Other names: cis-2,3-Epoxybicyclo[2.2.1]heptane
Inchi: InChI=1S/C7H10O/c1-2-5-3-4(1)6-7(5)8-6/h4-7H,1-3H2/t4?,5?,6-,7+
InchiKey: OHNNZOOGWXZCPZ-CYDAGYADSA-N
Formula: C7H10O
SMILES: C1CC2CC1C1OC21
Mol. weight [g/mol]: 110.15
CAS: 278-74-0

Physical Properties

Property code	Value	Unit	Source
chs	-4085.70	kJ/mol	NIST Webbook
gf	108.58	kJ/mol	Joback Method
hf	-53.90 ± 2.60	kJ/mol	NIST Webbook
hfs	-98.00 ± 2.50	kJ/mol	NIST Webbook
hfus	19.44	kJ/mol	Joback Method
hsub	44.10 ± 0.50	kJ/mol	NIST Webbook
hsub	44.10	kJ/mol	NIST Webbook
hvap	34.94	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.184		Crippen Method
mcvol	82.780	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	397.79	K	Joback Method
tc	601.21	K	Joback Method
tf	248.32	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.84	J/mol×K	397.79	Joback Method
cpg	193.57	J/mol×K	431.69	Joback Method
cpg	208.09	J/mol×K	465.60	Joback Method
cpg	221.49	J/mol×K	499.50	Joback Method

cpg	233.86	J/mol×K	533.40	Joback Method
cpg	245.27	J/mol×K	567.31	Joback Method
cpg	255.82	J/mol×K	601.21	Joback Method
dvisc	0.0002994	Pa×s	248.32	Joback Method
dvisc	0.0004034	Pa×s	273.23	Joback Method
dvisc	0.0005172	Pa×s	298.14	Joback Method
dvisc	0.0006381	Pa×s	323.05	Joback Method
dvisc	0.0007639	Pa×s	347.97	Joback Method
dvisc	0.0008928	Pa×s	372.88	Joback Method
dvisc	0.0010233	Pa×s	397.79	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=C278740&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume