cis-Bicyclo[4.1.0]hept-3-ene

Inchi: InChI=1S/C7H10/c1-2-4-7-5-6(7)3-1/h1-2,6-7H,3-5H2/t6-,7+
InchiKey: JBFDZEJAJZJORO-KNVOCYPGSA-N
Formula: C7H10
SMILES: C1=CCC2CC2C1
Mol. weight [g/mol]: 94.15
CAS: 16554-83-9

Physical Properties

Property code	Value	Unit	Source
gf	147.42	kJ/mol	Joback Method
hf	120.00	kJ/mol	NIST Webbook
hfus	9.28	kJ/mol	Joback Method
hvap	38.40 ± 0.60	kJ/mol	NIST Webbook
log10ws	-1.91		Crippen Method
logp	1.973		Crippen Method
mcvol	83.470	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
tb	376.47	K	Joback Method
tc	581.59	K	Joback Method
tf	201.77	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.52	J/mol×K	581.59	Joback Method
cpg	213.06	J/mol×K	547.41	Joback Method
cpg	201.82	J/mol×K	513.22	Joback Method
cpg	189.74	J/mol×K	479.03	Joback Method
cpg	176.76	J/mol×K	444.84	Joback Method
cpg	162.81	J/mol×K	410.66	Joback Method
cpg	147.84	J/mol×K	376.47	Joback Method
dvisc	0.0004629	Pa×s	201.77	Joback Method
dvisc	0.0004074	Pa×s	376.47	Joback Method

dvisc	0.0004125	Pa×s	347.35	Joback Method
dvisc	0.0004186	Pa×s	318.24	Joback Method
dvisc	0.0004260	Pa×s	289.12	Joback Method
dvisc	0.0004352	Pa×s	260.00	Joback Method
dvisc	0.0004471	Pa×s	230.89	Joback Method
hvapt	36.70	kJ/mol	358.50	NIST Webbook

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=C16554839&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
hvapt: Enthalpy of vaporization at a given temperature
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