Bicyclo[2.2.1]hept-2-ene,5-bromo-,endo-

Inchi: InChI=1S/C7H9Br/c8-7-4-5-1-2-6(7)3-5/h1-2,5-7H,3-4H2/t5?,6?,7-/m1/s1
InchiKey: DWPPXNJBRSZQHD-KPGICGJXSA-N
Formula: C7H9Br
SMILES: BrC1CC2C=CC1C2
Mol. weight [g/mol]: 173.05
CAS: 5810-82-2

Physical Properties

Property code	Value	Unit	Source
gf	154.03	kJ/mol	Joback Method
hf	15.40	kJ/mol	Joback Method
hfus	15.63	kJ/mol	Joback Method
hvap	37.59	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.346		Crippen Method
mcvol	100.970	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	437.96	K	Joback Method
tc	663.74	K	Joback Method
tf	257.33	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.71	J/mol×K	437.96	Joback Method
cpg	205.19	J/mol×K	475.59	Joback Method
cpg	218.54	J/mol×K	513.22	Joback Method
cpg	230.86	J/mol×K	550.85	Joback Method
cpg	242.21	J/mol×K	588.48	Joback Method
cpg	252.68	J/mol×K	626.11	Joback Method
cpg	262.35	J/mol×K	663.74	Joback Method
dvisc	0.0009362	Pa×s	257.33	Joback Method

dvisc	0.0009016	Pa×s	287.44	Joback Method
dvisc	0.0008745	Pa×s	317.54	Joback Method
dvisc	0.0008527	Pa×s	347.64	Joback Method
dvisc	0.0008348	Pa×s	377.75	Joback Method
dvisc	0.0008198	Pa×s	407.86	Joback Method
dvisc	0.0008071	Pa×s	437.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5810822&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
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
ie:	Ionization energy
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