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

Inchi: InChI=1S/C8H11Br/c9-5-8-4-6-1-2-7(8)3-6/h1-2,6-8H,3-5H2
InchiKey: XCDJEPZLSGMJSM-UHFFFAOYSA-N
Formula: C8H11Br
SMILES: BrCC1CC2C=CC1C2
Mol. weight [g/mol]: 187.08

Physical Properties

Property code	Value	Unit	Source
gf	162.45	kJ/mol	Joback Method
hf	-5.24	kJ/mol	Joback Method
hfus	18.22	kJ/mol	Joback Method
hvap	39.82	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.593		Crippen Method
mcvol	115.060	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	460.84	K	Joback Method
tc	683.28	K	Joback Method
tf	268.60	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.13	J/mol×K	460.84	Joback Method
cpg	247.61	J/mol×K	497.91	Joback Method
cpg	261.95	J/mol×K	534.99	Joback Method
cpg	275.23	J/mol×K	572.06	Joback Method
cpg	287.52	J/mol×K	609.13	Joback Method
cpg	298.91	J/mol×K	646.21	Joback Method
cpg	309.48	J/mol×K	683.28	Joback Method
dvisc	0.0011601	Pa×s	268.60	Joback Method

dvisc	0.0010773	Pa×s	300.64	Joback Method
dvisc	0.0010147	Pa×s	332.68	Joback Method
dvisc	0.0009659	Pa×s	364.72	Joback Method
dvisc	0.0009268	Pa×s	396.76	Joback Method
dvisc	0.0008947	Pa×s	428.80	Joback Method
dvisc	0.0008681	Pa×s	460.84	Joback Method

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=U381695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume