

Bicyclo[2.2.1]hept-5-ene, exo-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	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
tb	460.84	K	Joback Method
tc	683.28	K	Joback Method
tf	268.60	K	Joback Method
vc	0.436	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0010773	Paxs	300.64	Joback Method
dvisc	0.0010147	Paxs	332.68	Joback Method
dvisc	0.0009659	Paxs	364.72	Joback Method
dvisc	0.0009268	Paxs	396.76	Joback Method
dvisc	0.0008947	Paxs	428.80	Joback Method
dvisc	0.0008681	Paxs	460.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U381694&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
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

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