

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

Inchi:	InChI=1S/C7H9Br/c8-7-4-5-1-2-6(7)3-5/h1-2,5-7H,3-4H2/t5?,6?,7-/m0/s1
InchiKey:	DWPPXNJBRSZQHD-AHXFUIDQSA-N
Formula:	C7H9Br
SMILES:	BrC1CC2C=CC1C2
Mol. weight [g/mol]:	173.05
CAS:	5889-54-3

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.71	J/molxK	437.96	Joback Method
cpg	252.68	J/molxK	626.11	Joback Method
cpg	242.21	J/molxK	588.48	Joback Method
cpg	230.86	J/molxK	550.85	Joback Method
cpg	218.54	J/molxK	513.22	Joback Method
cpg	205.19	J/molxK	475.59	Joback Method
cpg	262.35	J/molxK	663.74	Joback Method
dvisc	0.0008071	Paxs	437.96	Joback Method

dvisc	0.0008198	Paxs	407.86	Joback Method
dvisc	0.0008348	Paxs	377.75	Joback Method
dvisc	0.0008527	Paxs	347.64	Joback Method
dvisc	0.0008745	Paxs	317.54	Joback Method
dvisc	0.0009016	Paxs	287.44	Joback Method
dvisc	0.0009362	Paxs	257.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5889543&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
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

Latest version available from:

<https://www.chemeo.com/cid/61-559-4/Bicyclo-2-2-1-hept-2-ene-5-bromo-exo.pdf>

Generated by Cheméo on 2024-04-19 20:55:39.106515542 +0000 UTC m=+15849388.027092855.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.