Bicyclo[4.2.0]octa-1,3,5-triene, 7-bromo-

Other names: 1-bromobenzocyclobutene
Inchi: InChI=1S/C8H7Br/c9-8-5-6-3-1-2-4-7(6)8/h1-4,8H,5H2
InchiKey: AYNXHFRDABNHRX-UHFFFAOYSA-N
Formula: C8H7Br
SMILES: BrC1Cc2ccccc21
Mol. weight [g/mol]: 183.04
CAS: 21120-91-2

Physical Properties

Property code	Value	Unit	Source
gf	206.43	kJ/mol	Joback Method
hf	121.90	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	42.52	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.679		Crippen Method
mcvol	106.460	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	482.73	K	Joback Method
tc	722.52	K	Joback Method
tf	300.12	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.50	J/mol×K	482.73	Joback Method
cpg	210.28	J/mol×K	522.70	Joback Method
cpg	221.02	J/mol×K	562.66	Joback Method
cpg	230.82	J/mol×K	602.63	Joback Method
cpg	239.77	J/mol×K	642.59	Joback Method
cpg	247.97	J/mol×K	682.56	Joback Method
cpg	255.51	J/mol×K	722.52	Joback Method
dvisc	0.0014198	Pa×s	300.12	Joback Method

dvisc	0.0011806	Pa×s	330.56	Joback Method
dvisc	0.0010127	Pa×s	360.99	Joback Method
dvisc	0.0008896	Pa×s	391.42	Joback Method
dvisc	0.0007963	Pa×s	421.86	Joback Method
dvisc	0.0007235	Pa×s	452.29	Joback Method
dvisc	0.0006653	Pa×s	482.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21120912&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
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