

7-Bromo-1,3,5-cyclooctatriene

Inchi:	InChI=1S/C8H9Br/c9-8-6-4-2-1-3-5-7-8/h1-6,8H,7H2/b2-1-,5-3-,6-4-
InchiKey:	CJZXWYXQEJTDRN-XCADPSHZSA-N
Formula:	C8H9Br
SMILES:	BrC1C=CC=CC=CC1
Mol. weight [g/mol]:	185.06
CAS:	16327-13-2

Physical Properties

Property code	Value	Unit	Source
gf	120.93	kJ/mol	Joback Method
hf	33.22	kJ/mol	Joback Method
hfus	13.06	kJ/mol	Joback Method
hvap	41.49	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.822		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	474.17	K	Joback Method
tc	720.01	K	Joback Method
tf	242.34	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.98	J/molxK	474.17	Joback Method
cpg	227.05	J/molxK	515.14	Joback Method
cpg	241.08	J/molxK	556.12	Joback Method
cpg	254.12	J/molxK	597.09	Joback Method
cpg	266.18	J/molxK	638.06	Joback Method
cpg	277.31	J/molxK	679.04	Joback Method
cpg	287.53	J/molxK	720.01	Joback Method
dvisc	0.0059430	Paxs	242.34	Joback Method
dvisc	0.0023806	Paxs	280.98	Joback Method

dvisc	0.0011897	Paxs	319.62	Joback Method
dvisc	0.0006905	Paxs	358.25	Joback Method
dvisc	0.0004456	Paxs	396.89	Joback Method
dvisc	0.0003107	Paxs	435.53	Joback Method
dvisc	0.0002298	Paxs	474.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16327132&Units=SI
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

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

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