Cyclooctyl bromide

Other names: Cyclooctane, bromo-
Bromocyclooctane
Inchi: InChI=1S/C8H15Br/c9-8-6-4-2-1-3-5-7-8/h8H,1-7H2
InchiKey: KFKLBMQLKLKHLU-UHFFFAOYSA-N
Formula: C8H15Br
SMILES: BrC1CCCCCCC1
Mol. weight [g/mol]: 191.11
CAS: 1556-09-8

Physical Properties

Property code	Value	Unit	Source
gf	31.05	kJ/mol	Joback Method
hf	-140.12	kJ/mol	Joback Method
hfus	9.40	kJ/mol	Joback Method
hvap	40.61	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.494		Crippen Method
mcvol	130.220	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
tb	476.69	K	Joback Method
tc	714.64	K	Joback Method
tf	240.06	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.64	J/mol×K	476.69	Joback Method
cpg	278.98	J/mol×K	516.35	Joback Method
cpg	297.15	J/mol×K	556.01	Joback Method
cpg	314.21	J/mol×K	595.66	Joback Method

cpg	330.16	J/mol×K	635.32	Joback Method
cpg	345.04	J/mol×K	674.98	Joback Method
cpg	358.87	J/mol×K	714.64	Joback Method
dvisc	0.0121613	Pa×s	240.06	Joback Method
dvisc	0.0039819	Pa×s	279.50	Joback Method
dvisc	0.0017184	Pa×s	318.94	Joback Method
dvisc	0.0008922	Pa×s	358.38	Joback Method
dvisc	0.0005276	Pa×s	397.81	Joback Method
dvisc	0.0003429	Pa×s	437.25	Joback Method
dvisc	0.0002394	Pa×s	476.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1556098&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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