Bicyclo[3.3.0]octane, 2-bromo-6-(trichloromethyl)

Inchi: InChI=1S/C9H12Br4/c10-8-4-2-5-6(8)1-3-7(5)9(11,12)13/h5-8H,1-4H2
InchiKey: IMPUYTHHLICXRH-UHFFFAOYSA-N
Formula: C9H12Br4
SMILES: BrC1CCC2C1CCC2C(Br)(Br)Br
Mol. weight [g/mol]: 439.81

Physical Properties

Property code	Value	Unit	Source
gf	166.90	kJ/mol	Joback Method
hf	-39.92	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	59.62	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.025		Crippen Method
mcvol	185.950	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1702.00		NIST Webbook
tb	679.41	K	Joback Method
tc	963.18	K	Joback Method
tf	453.17	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.69	J/mol×K	679.41	Joback Method
cpg	433.33	J/mol×K	726.70	Joback Method
cpg	446.54	J/mol×K	774.00	Joback Method
cpg	458.58	J/mol×K	821.29	Joback Method
cpg	469.69	J/mol×K	868.59	Joback Method
cpg	480.12	J/mol×K	915.88	Joback Method
cpg	490.12	J/mol×K	963.18	Joback Method
dvisc	0.0025360	Pa×s	453.17	Joback Method
dvisc	0.0019877	Pa×s	490.88	Joback Method

dvisc	0.0016130	Pa×s	528.58	Joback Method
dvisc	0.0013459	Pa×s	566.29	Joback Method
dvisc	0.0011487	Pa×s	604.00	Joback Method
dvisc	0.0009988	Pa×s	641.70	Joback Method
dvisc	0.0008821	Pa×s	679.41	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=R515256&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