Bromopentachloroethane

Inchi: InChI=1S/C2BrCl5/c3-1(4,5)2(6,7)8
InchiKey: YVDACVUIWDTEJU-UHFFFAOYSA-N
Formula: C2BrCl5
SMILES: ClC(Cl)(Cl)C(Cl)(Cl)Br
Mol. weight [g/mol]: 281.19
CAS: 79504-02-2

Physical Properties

Property code	Value	Unit	Source
gf	-73.69	kJ/mol	Joback Method
hf	-154.48	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	45.81	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.883		Crippen Method
mcvol	117.740	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
tb	492.01	K	Joback Method
tc	752.13	K	Joback Method
tf	326.54	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.72	J/mol×K	752.13	Joback Method
cpg	173.06	J/mol×K	708.78	Joback Method
cpg	172.02	J/mol×K	665.42	Joback Method
cpg	170.49	J/mol×K	622.07	Joback Method
cpg	168.34	J/mol×K	578.72	Joback Method
cpg	165.47	J/mol×K	535.36	Joback Method
cpg	161.75	J/mol×K	492.01	Joback Method
dvisc	0.0038453	Pa×s	326.54	Joback Method
dvisc	0.0004326	Pa×s	492.01	Joback Method

dvisc	0.0005589	Pa×s	464.43	Joback Method
dvisc	0.0007456	Pa×s	436.85	Joback Method
dvisc	0.0010342	Pa×s	409.27	Joback Method
dvisc	0.0015040	Pa×s	381.70	Joback Method
dvisc	0.0023185	Pa×s	354.12	Joback Method
hsubt	44.40	kJ/mol	408.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48630e+01
Coeff. B	-5.34200e+03
Temperature range (K), min.	366.51
Temperature range (K), max.	559.29

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C79504022&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
hsubt: Enthalpy of sublimation at a given temperature
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume