Cyclopentanol, 2-bromo-, trans-

Other names:	trans-2-Bromocyclopentanol
	2-Bromocyclopentanol, (E)-
Inchi:	InChI=1S/C5H9BrO/c6-4-2-1-3-5(4)7/h4-5,7H,1-3H2/t4-,5-/m1/s1
InchiKey:	BQVWZYQFAVLQKE-RFZPGFLSSA-N
Formula:	C5H9BrO
SMILES:	OC1CCCC1Br
Mol. weight [g/mol]:	165.03
CAS:	20377-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-102.44	kJ/mol	Joback Method
hf	-232.29	kJ/mol	Joback Method
hfus	13.08	kJ/mol	Joback Method
hvap	49.79	kJ/mol	Joback Method
ie	10.11 ± 0.02	eV	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.295		Crippen Method
mcvol	93.820	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
tb	482.75	K	Joback Method
tc	688.92	K	Joback Method
tf	273.39	K	Joback Method
vc	0.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.36	J/mol×K	482.75	Joback Method
cpg	198.08	J/mol×K	517.11	Joback Method
cpg	208.18	J/mol×K	551.47	Joback Method
cpg	217.68	J/mol×K	585.84	Joback Method
cpg	226.62	J/mol×K	620.20	Joback Method
cpg	235.02	J/mol×K	654.56	Joback Method

cpg	242.91	J/mol×K	688.92	Joback Method
dvisc	0.0161533	Pa×s	273.39	Joback Method
dvisc	0.0058608	Pa×s	308.28	Joback Method
dvisc	0.0026133	Pa×s	343.18	Joback Method
dvisc	0.0013526	Pa×s	378.07	Joback Method
dvisc	0.0007825	Pa×s	412.96	Joback Method
dvisc	0.0004930	Pa×s	447.86	Joback Method
dvisc	0.0003320	Pa×s	482.75	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=C20377791&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
ie: Ionization energy
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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