trans-2-bromocyclohexanol

Other names: 2-Bromocyclohexanol, (E)
trans-2-Bromocyclohexanol
Inchi: InChI=1S/C6H11BrO/c7-5-3-1-2-4-6(5)8/h5-6,8H,1-4H2
InchiKey: AAMCLCZHZXKWRV-UHFFFAOYSA-N
Formula: C6H11BrO
SMILES: OC1CCCCC1Br
Mol. weight [g/mol]: 179.06

Physical Properties

Property code	Value	Unit	Source
hf	-242.81	kJ/mol	Cheméo Relay (1.0)
hfus	13.57	kJ/mol	Joback Method
hvap	71.70	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
logp	1.685		Crippen Method
mcvol	107.910	ml/mol	McGowan Method
tb	484.60	K	Cheméo Relay (1.0)
tf	294.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.93	J/mol×K	509.90	Joback Method
cpg	241.56	J/mol×K	545.04	Joback Method
cpg	253.47	J/mol×K	580.19	Joback Method
cpg	264.69	J/mol×K	615.33	Joback Method
cpg	275.23	J/mol×K	650.48	Joback Method
cpg	285.13	J/mol×K	685.62	Joback Method
cpg	294.40	J/mol×K	720.76	Joback Method
dvisc	0.0184055	Pa×s	281.14	Joback Method
dvisc	0.0057078	Pa×s	319.27	Joback Method
dvisc	0.0022724	Pa×s	357.39	Joback Method
dvisc	0.0010805	Pa×s	395.52	Joback Method
dvisc	0.0005855	Pa×s	433.65	Joback Method

dvisc	0.0003503	Pa×s	471.77	Joback Method
dvisc	0.0002263	Pa×s	509.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2425334&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point