Hexabromoethane

Other names: Hexabromoethane
Inchi: InChI=1S/C2Br6/c3-1(4,5)2(6,7)8
InchiKey: POJPQMDDRCILHJ-UHFFFAOYSA-N
Formula: C2Br6
SMILES: BrC(Br)(Br)C(Br)(Br)Br
Mol. weight [g/mol]: 503.45

Physical Properties

Property code	Value	Unit	Source
hf	133.00	kJ/mol	NIST Webbook
hfus	17.82	kJ/mol	Joback Method
ie	10.20	eV	Cheméo Relay (1.0)
log10ws	-5.08		Cheméo Relay (1.0)
logp	4.663		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
tf	427.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.53	J/mol×K	635.66	Joback Method
cpg	178.35	J/mol×K	955.52	Joback Method
cpg	177.43	J/mol×K	902.21	Joback Method
cpg	177.20	J/mol×K	848.90	Joback Method
cpg	177.32	J/mol×K	795.59	Joback Method
cpg	177.46	J/mol×K	742.28	Joback Method
cpg	177.31	J/mol×K	688.97	Joback Method
dvisc	0.0004276	Pa×s	555.80	Joback Method
dvisc	0.0002329	Pa×s	635.66	Joback Method
dvisc	0.0002802	Pa×s	609.04	Joback Method
dvisc	0.0003428	Pa×s	582.42	Joback Method
dvisc	0.0009628	Pa×s	475.94	Joback Method
dvisc	0.0005454	Pa×s	529.18	Joback Method
dvisc	0.0007138	Pa×s	502.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594730&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point