5-Methyl-2,3-dibromohexane

Inchi: InChI=1S/C7H14Br2/c1-5(2)4-7(9)6(3)8/h5-7H,4H2,1-3H3
InchiKey: RKFQBBTZZFOSGZ-UHFFFAOYSA-N
Formula: C7H14Br2
SMILES: CC(C)CC(Br)C(C)Br
Mol. weight [g/mol]: 257.99

Physical Properties

Property code	Value	Unit	Source
gf	29.38	kJ/mol	Joback Method
hf	-150.99	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	42.88	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.579		Crippen Method
mcvol	144.490	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
tb	490.56	K	Joback Method
tc	703.38	K	Joback Method
tf	243.25	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.94	J/mol×K	490.56	Joback Method
cpg	288.45	J/mol×K	526.03	Joback Method
cpg	300.23	J/mol×K	561.50	Joback Method
cpg	311.32	J/mol×K	596.97	Joback Method
cpg	321.75	J/mol×K	632.44	Joback Method
cpg	331.56	J/mol×K	667.91	Joback Method
cpg	340.79	J/mol×K	703.38	Joback Method
dvisc	0.0088592	Pa×s	243.25	Joback Method

dvisc	0.0033104	Pa×s	284.47	Joback Method
dvisc	0.0015870	Pa×s	325.69	Joback Method
dvisc	0.0008975	Pa×s	366.90	Joback Method
dvisc	0.0005695	Pa×s	408.12	Joback Method
dvisc	0.0003928	Pa×s	449.34	Joback Method
dvisc	0.0002884	Pa×s	490.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559454&Units=SI
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

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