3-Methyl-2,3-dibromopentane

Inchi: InChI=1S/C6H12Br2/c1-4-6(3,8)5(2)7/h5H,4H2,1-3H3
InchiKey: VYEPHBKIORGLPY-UHFFFAOYSA-N
Formula: C6H12Br2
SMILES: CCC(C)(Br)C(C)Br
Mol. weight [g/mol]: 243.97

Physical Properties

Property code	Value	Unit	Source
gf	28.68	kJ/mol	Joback Method
hf	-128.54	kJ/mol	Joback Method
hfus	10.93	kJ/mol	Joback Method
hvap	40.14	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.333		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1084.00		NIST Webbook
tb	465.33	K	Joback Method
tc	685.60	K	Joback Method
tf	264.40	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.33	J/mol×K	465.33	Joback Method
cpg	288.43	J/mol×K	648.89	Joback Method
cpg	279.70	J/mol×K	612.18	Joback Method
cpg	270.28	J/mol×K	575.46	Joback Method
cpg	260.11	J/mol×K	538.75	Joback Method
cpg	249.15	J/mol×K	502.04	Joback Method
cpg	296.54	J/mol×K	685.60	Joback Method
dvisc	0.0003564	Pa×s	465.33	Joback Method

dvisc	0.0004749	Pa×s	431.84	Joback Method
dvisc	0.0006643	Pa×s	398.35	Joback Method
dvisc	0.0009880	Pa×s	364.87	Joback Method
dvisc	0.0015925	Pa×s	331.38	Joback Method
dvisc	0.0028574	Pa×s	297.89	Joback Method
dvisc	0.0059456	Pa×s	264.40	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=R559305&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
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