3,4-Dimethyl-2,3-dibromopentane

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

Physical Properties

Property code	Value	Unit	Source
gf	34.66	kJ/mol	Joback Method
hf	-154.46	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	41.97	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.579		Crippen Method
mcvol	144.490	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	1126.00		NIST Webbook
tb	487.77	K	Joback Method
tc	709.79	K	Joback Method
tf	260.67	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.91	J/mol×K	487.77	Joback Method
cpg	292.19	J/mol×K	524.77	Joback Method
cpg	304.52	J/mol×K	561.78	Joback Method
cpg	315.97	J/mol×K	598.78	Joback Method
cpg	326.61	J/mol×K	635.78	Joback Method
cpg	336.49	J/mol×K	672.78	Joback Method
cpg	345.67	J/mol×K	709.79	Joback Method
dvisc	0.0082082	Pa×s	260.67	Joback Method
dvisc	0.0033291	Pa×s	298.52	Joback Method

dvisc	0.0016543	Pa×s	336.37	Joback Method
dvisc	0.0009469	Pa×s	374.22	Joback Method
dvisc	0.0006006	Pa×s	412.07	Joback Method
dvisc	0.0004112	Pa×s	449.92	Joback Method
dvisc	0.0002986	Pa×s	487.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559414&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

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