

4-Methyl-2,3-dibromopentane

Inchi:	InChI=1S/C6H12Br2/c1-4(2)6(8)5(3)7/h4-6H,1-3H3
InchiKey:	BLKGASDZOMDLNX-UHFFFAOYSA-N
Formula:	C6H12Br2
SMILES:	CC(C)C(Br)C(C)Br
Mol. weight [g/mol]:	243.97

Physical Properties

Property code	Value	Unit	Source
gf	20.96	kJ/mol	Joback Method
hf	-130.35	kJ/mol	Joback Method
hfus	11.30	kJ/mol	Joback Method
hvap	40.66	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.189		Crippen Method
mvol	130.400	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1075.00		NIST Webbook
tb	467.68	K	Joback Method
tc	683.72	K	Joback Method
tf	231.98	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.62	J/molxK	467.68	Joback Method
cpg	246.00	J/molxK	503.69	Joback Method
cpg	256.68	J/molxK	539.69	Joback Method
cpg	266.73	J/molxK	575.70	Joback Method
cpg	276.16	J/molxK	611.71	Joback Method
cpg	285.01	J/molxK	647.72	Joback Method
cpg	293.33	J/molxK	683.72	Joback Method
dvisc	0.0094755	Paxs	231.98	Joback Method

dvisc	0.0035817	Paxs	271.26	Joback Method
dvisc	0.0017317	Paxs	310.55	Joback Method
dvisc	0.0009857	Paxs	349.83	Joback Method
dvisc	0.0006287	Paxs	389.11	Joback Method
dvisc	0.0004354	Paxs	428.40	Joback Method
dvisc	0.0003208	Paxs	467.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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