

Hexane, 1,2,5,6-tetrabromo-

Other names:	1,2,5,6-Tetrabromohexane
Inchi:	InChI=1S/C6H10Br4/c7-3-5(9)1-2-6(10)4-8/h5-6H,1-4H2
InchiKey:	WPBWUVCMCYXPI-UHFFFAOYSA-N
Formula:	C6H10Br4
SMILES:	BrCC(Br)CCC(Br)CBr
Mol. weight [g/mol]:	401.76
CAS:	58443-86-0

Physical Properties

Property code	Value	Unit	Source
gf	52.04	kJ/mol	Joback Method
hf	-72.41	kJ/mol	Joback Method
hfus	25.39	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.083		Crippen Method
mcvol	165.400	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	600.44	K	Joback Method
tc	841.15	K	Joback Method
tf	322.65 ± 2.00	K	NIST Webbook
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.17	J/mol×K	600.44	Joback Method
cpg	307.26	J/mol×K	640.56	Joback Method
cpg	315.64	J/mol×K	680.68	Joback Method
cpg	323.40	J/mol×K	720.80	Joback Method
cpg	330.60	J/mol×K	760.92	Joback Method
cpg	337.33	J/mol×K	801.03	Joback Method
cpg	343.65	J/mol×K	841.15	Joback Method
dvisc	0.0022919	Pa×s	366.58	Joback Method

dvisc	0.0013250	Pa×s	405.56	Joback Method
dvisc	0.0008433	Pa×s	444.53	Joback Method
dvisc	0.0005772	Pa×s	483.51	Joback Method
dvisc	0.0004181	Pa×s	522.49	Joback Method
dvisc	0.0003167	Pa×s	561.46	Joback Method
dvisc	0.0002487	Pa×s	600.44	Joback Method

Sources

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=C58443860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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