Hexane, 1,2-dibromo-

Other names: 1,2-Dibromohexane
Inchi: InChI=1S/C6H12Br2/c1-2-3-4-6(8)5-7/h6H,2-5H2,1H3
InchiKey: NUUUANNAZVEWHM-UHFFFAOYSA-N
Formula: C6H12Br2
SMILES: CCCCC(Br)CBr
Mol. weight [g/mol]: 243.97
CAS: 624-20-4

Physical Properties

Property code	Value	Unit	Source
gf	25.84	kJ/mol	Joback Method
hf	-119.79	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	56.50 ± 2.00	kJ/mol	NIST Webbook
log10ws	-3.31		Crippen Method
logp	3.335		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
tb	360.15 ± 0.50	K	NIST Webbook
tc	674.72	K	Joback Method
tf	261.98	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.23	J/mol×K	468.56	Joback Method
cpg	281.92	J/mol×K	640.36	Joback Method
cpg	273.46	J/mol×K	606.00	Joback Method
cpg	264.50	J/mol×K	571.64	Joback Method

cpg	254.99	J/mol×K	537.28	Joback Method
cpg	244.92	J/mol×K	502.92	Joback Method
cpg	289.89	J/mol×K	674.72	Joback Method
dvisc	0.0003546	Pa×s	468.56	Joback Method
dvisc	0.0004558	Pa×s	434.13	Joback Method
dvisc	0.0006117	Pa×s	399.70	Joback Method
dvisc	0.0008678	Pa×s	365.27	Joback Method
dvisc	0.0013240	Pa×s	330.84	Joback Method
dvisc	0.0022284	Pa×s	296.41	Joback Method
dvisc	0.0043004	Pa×s	261.98	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50293e+01
Coeff. B	-4.23677e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	360.92
Temperature range (K), max.	509.50

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=C624204&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume