

1,5-dibromohexane

Inchi:	InChI=1S/C6H12Br2/c1-6(8)4-2-3-5-7/h6H,2-5H2,1H3
InchiKey:	FINUUDAOCYEWBV-UHFFFAOYSA-N
Formula:	C6H12Br2
SMILES:	CC(Br)CCCCBr
Mol. weight [g/mol]:	243.97
CAS:	627-96-3

Physical Properties

Property code	Value	Unit	Source
af	0.5192		Cheméo Relay (1.0)
hf	-153.49	kJ/mol	Cheméo Relay (1.0)
hfus	18.34	kJ/mol	Joback Method
hvap	54.99	kJ/mol	Cheméo Relay (1.0)
ie	9.88	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	3.335		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	489.80	K	Cheméo Relay (1.0)
tc	678.28	K	Cheméo Relay (1.0)
tf	239.19	K	Cheméo Relay (1.0)
vc	0.465	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.23	J/mol×K	468.56	Joback Method
cpg	244.92	J/mol×K	502.92	Joback Method
cpg	254.99	J/mol×K	537.28	Joback Method
cpg	264.50	J/mol×K	571.64	Joback Method
cpg	273.46	J/mol×K	606.00	Joback Method
cpg	281.92	J/mol×K	640.36	Joback Method
cpg	289.89	J/mol×K	674.72	Joback Method
dvisc	0.0043004	Pa×s	261.98	Joback Method

dvisc	0.0022284	Pa×s	296.41	Joback Method
dvisc	0.0013240	Pa×s	330.84	Joback Method
dvisc	0.0008678	Pa×s	365.27	Joback Method
dvisc	0.0006117	Pa×s	399.70	Joback Method
dvisc	0.0004558	Pa×s	434.13	Joback Method
dvisc	0.0003546	Pa×s	468.56	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53005e+01
Coeff. B	-4.33821e+03
Coeff. C	-7.43540e+01
Temperature range (K), min.	363.32
Temperature range (K), max.	508.65

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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