Hexane, 2,5-dibromo-

Other names: 2,5-Dibromohexane
Inchi: InChI=1S/C6H12Br2/c1-5(7)3-4-6(2)8/h5-6H,3-4H2,1-2H3
InchiKey: MQYLGFBWOZXHHF-UHFFFAOYSA-N
Formula: C6H12Br2
SMILES: CC(Br)CCC(C)Br
Mol. weight [g/mol]: 243.97
CAS: 24774-58-1

Physical Properties

Property code	Value	Unit	Source
gf	23.40	kJ/mol	Joback Method
hf	-125.07	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	41.04	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.333		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	481.15 ± 5.00	K	NIST Webbook
tc	679.14	K	Joback Method
tf	311.15 ± 2.00	K	NIST Webbook
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.43	J/mol×K	468.12	Joback Method
cpg	245.45	J/mol×K	503.29	Joback Method
cpg	255.83	J/mol×K	538.46	Joback Method
cpg	265.60	J/mol×K	573.63	Joback Method
cpg	274.79	J/mol×K	608.80	Joback Method
cpg	283.45	J/mol×K	643.97	Joback Method
cpg	291.59	J/mol×K	679.14	Joback Method
dvisc	0.0061816	Pa×s	246.98	Joback Method

dvisc	0.0027790	Pa×s	283.84	Joback Method
dvisc	0.0015014	Pa×s	320.69	Joback Method
dvisc	0.0009209	Pa×s	357.55	Joback Method
dvisc	0.0006189	Pa×s	394.41	Joback Method
dvisc	0.0004452	Pa×s	431.26	Joback Method
dvisc	0.0003373	Pa×s	468.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54241e+01
Coeff. B	-4.38975e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	364.92
Temperature range (K), max.	508.99

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24774581&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

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