Pentane, 1,3-dibromo-

Other names:	1,3-Dibromopentane
Inchi:	InChI=1S/C5H10Br2/c1-2-5(7)3-4-6/h5H,2-4H2,1H3
InchiKey:	SOZLNIPBRVQUOG-UHFFFAOYSA-N
Formula:	C5H10Br2
SMILES:	CCC(Br)CCBr
Mol. weight [g/mol]:	229.94
CAS:	42474-20-4

Physical Properties

Property code	Value	Unit	Source
gf	17.42	kJ/mol	Joback Method
hf	-99.15	kJ/mol	Joback Method
hfl	-170.80	kJ/mol	NIST Webbook
hfus	15.75	kJ/mol	Joback Method
hvap	39.21	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.945		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	445.68	K	Joback Method
tc	654.58	K	Joback Method
tf	250.71	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.09	J/mol×K	445.68	Joback Method
cpg	204.52	J/mol×K	480.50	Joback Method
cpg	213.39	J/mol×K	515.31	Joback Method
cpg	221.74	J/mol×K	550.13	Joback Method
cpg	229.60	J/mol×K	584.95	Joback Method
cpg	237.00	J/mol×K	619.76	Joback Method
cpg	243.97	J/mol×K	654.58	Joback Method

dvisc	0.0043813	Pa×s	250.71	Joback Method
dvisc	0.0023206	Pa×s	283.20	Joback Method
dvisc	0.0014009	Pa×s	315.70	Joback Method
dvisc	0.0009293	Pa×s	348.19	Joback Method
dvisc	0.0006612	Pa×s	380.69	Joback Method
dvisc	0.0004963	Pa×s	413.19	Joback Method
dvisc	0.0003884	Pa×s	445.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55046e+01
Coeff. B	-4.27012e+03
Coeff. C	-6.99060e+01
Temperature range (K), min.	350.52
Temperature range (K), max.	488.83

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42474204&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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