1,2-Dibromopentane

Other names: Pentane, 1,2-dibromo-
Inchi: InChI=1S/C5H10Br2/c1-2-3-5(7)4-6/h5H,2-4H2,1H3
InchiKey: CITMYAPULDSOHG-UHFFFAOYSA-N
Formula: C5H10Br2
SMILES: CCCC(Br)CBr
Mol. weight [g/mol]: 229.94
CAS: 3234-49-9

Physical Properties

Property code	Value	Unit	Source
gf	17.42	kJ/mol	Joback Method
hf	-99.15	kJ/mol	Joback Method
hfl	-164.80	kJ/mol	NIST Webbook
hfus	15.75	kJ/mol	Joback Method
hvap	49.00	kJ/mol	NIST Webbook
hvap	49.20 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.89		Crippen Method
logp	2.945		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1056.00		NIST Webbook
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	237.00	J/mol×K	619.76	Joback Method

cpg	243.97	J/mol×K	654.58	Joback Method
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
dvisc	0.0003884	Pa×s	445.68	Joback Method
dvisc	0.0004963	Pa×s	413.19	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
hvapt	48.80	kJ/mol	370.00	NIST Webbook
hvapt	46.50	kJ/mol	406.50	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3234499&Units=SI

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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume