1,2-dibromononane

Inchi: InChI=1S/C9H18Br2/c1-2-3-4-5-6-7-8-9(10)11/h9H,2-8H2,1H3
InchiKey: FSTKSTMFMLANPA-UHFFFAOYSA-N
Formula: C9H18Br2
SMILES: CCCCCCCCC(Br)Br
Mol. weight [g/mol]: 286.05
CAS: 73642-91-8

Physical Properties

Property code	Value	Unit	Source
af	0.6319		Cheméo Relay (1.0)
gf	51.10	kJ/mol	Joback Method
hf	-179.68	kJ/mol	Cheméo Relay (1.0)
hfus	26.11	kJ/mol	Joback Method
hvap	66.08	kJ/mol	Cheméo Relay (1.0)
ie	9.91	eV	Cheméo Relay (1.0)
log10ws	-5.68		Cheméo Relay (1.0)
logp	4.853		Crippen Method
mcvol	172.670	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	523.92	K	Cheméo Relay (1.0)
tc	711.37	K	Cheméo Relay (1.0)
tf	239.42	K	Cheméo Relay (1.0)
vc	0.645	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.78	J/mol×K	537.20	Joback Method
cpg	377.44	J/mol×K	570.16	Joback Method
cpg	390.37	J/mol×K	603.13	Joback Method
cpg	402.61	J/mol×K	636.09	Joback Method
cpg	414.20	J/mol×K	669.06	Joback Method
cpg	425.18	J/mol×K	702.02	Joback Method
cpg	435.58	J/mol×K	734.99	Joback Method

dvisc	0.0037768	Pa×s	295.79	Joback Method
dvisc	0.0018483	Pa×s	336.03	Joback Method
dvisc	0.0010539	Pa×s	376.26	Joback Method
dvisc	0.0006698	Pa×s	416.50	Joback Method
dvisc	0.0004611	Pa×s	456.73	Joback Method
dvisc	0.0003372	Pa×s	496.97	Joback Method
dvisc	0.0002585	Pa×s	537.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58928e+01
Coeff. B	-4.97370e+03
Coeff. C	-9.02000e+01
Temperature range (K), min.	408.92
Temperature range (K), max.	560.24

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C73642918&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor

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
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