1,7-DIBROMOHEPTANE

Other names:	Dibromo-1,7 heptane
	Heptamethylene dibromide
Inchi:	InChI=1S/C7H14Br2/c8-6-4-2-1-3-5-7-9/h1-7H2
InchiKey:	LVWSZGCVEZRFBT-UHFFFAOYSA-N
Formula:	C7H14Br2
SMILES:	BrCCCCCCCBr
Mol. weight [g/mol]:	258.00
CAS:	4549-31-9

Physical Properties

Property code	Value	Unit	Source
af	0.6181		Cheméo Relay (1.0)
gf	36.70	kJ/mol	Joback Method
hf	-162.75	kJ/mol	Cheméo Relay (1.0)
hfus	24.46	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Cheméo Relay (1.0)
ie	9.84	eV	Cheméo Relay (1.0)
log10ws	-4.85		Cheméo Relay (1.0)
logp	3.727		Crippen Method
mcvol	144.490	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1397.00		NIST Webbook
ripol	1863.00		NIST Webbook
tb	528.20	K	NIST Webbook
tb	528.00	K	NIST Webbook
tb	536.20	K	NIST Webbook
tc	700.75	K	Cheméo Relay (1.0)
tf	276.96	K	Cheméo Relay (1.0)
vc	0.535	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.23	J/mol×K	491.88	Joback Method
cpg	286.69	J/mol×K	525.03	Joback Method
cpg	297.54	J/mol×K	558.17	Joback Method
cpg	307.81	J/mol×K	591.32	Joback Method
cpg	317.52	J/mol×K	624.46	Joback Method
cpg	326.72	J/mol×K	657.61	Joback Method
cpg	335.42	J/mol×K	690.76	Joback Method
dvisc	0.0030933	Pa×s	288.25	Joback Method
dvisc	0.0017626	Pa×s	322.19	Joback Method
dvisc	0.0011180	Pa×s	356.13	Joback Method
dvisc	0.0007676	Pa×s	390.06	Joback Method
dvisc	0.0005597	Pa×s	424.00	Joback Method
dvisc	0.0004277	Pa×s	457.94	Joback Method
dvisc	0.0003392	Pa×s	491.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37785e+01
Coeff. B	-4.08857e+03
Coeff. C	-8.18600e+01
Temperature range (K), min.	384.92
Temperature range (K), max.	564.74

Sources

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=C4549319&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

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