Octane, 1,2-dibromo-

Other names: 1,2-Dibromooctane
Inchi: InChI=1S/C8H16Br2/c1-2-3-4-5-6-8(10)7-9/h8H,2-7H2,1H3
InchiKey: BJJLJKYBNCPTQS-UHFFFAOYSA-N
Formula: C8H16Br2
SMILES: CCCCCCC(Br)CBr
Mol. weight [g/mol]: 272.02
CAS: 6269-92-7

Physical Properties

Property code	Value	Unit	Source
gf	42.68	kJ/mol	Joback Method
hf	-161.07	kJ/mol	Joback Method
hfus	23.52	kJ/mol	Joback Method
hvap	45.88	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	4.115		Crippen Method
mcvol	158.580	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1335.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1226.00		NIST Webbook
tb	514.32	K	Joback Method
tc	714.87	K	Joback Method
tf	284.52	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.69	J/mol×K	514.32	Joback Method
cpg	331.47	J/mol×K	547.74	Joback Method
cpg	343.57	J/mol×K	581.17	Joback Method
cpg	355.01	J/mol×K	614.59	Joback Method
cpg	365.83	J/mol×K	648.02	Joback Method

cpg	376.07	J/mol×K	681.44	Joback Method
cpg	385.75	J/mol×K	714.87	Joback Method
dvisc	0.0039870	Pa×s	284.52	Joback Method
dvisc	0.0019862	Pa×s	322.82	Joback Method
dvisc	0.0011470	Pa×s	361.12	Joback Method
dvisc	0.0007360	Pa×s	399.42	Joback Method
dvisc	0.0005104	Pa×s	437.72	Joback Method
dvisc	0.0003754	Pa×s	476.02	Joback Method
dvisc	0.0002890	Pa×s	514.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57364e+01
Coeff. B	-4.77871e+03
Coeff. C	-8.51960e+01
Temperature range (K), min.	394.52
Temperature range (K), max.	543.59

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=C6269927&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
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