

3-Bromooctane

Other names:	Octane, 3-bromo-
Inchi:	InChI=1S/C8H17Br/c1-3-5-6-7-8(9)4-2/h8H,3-7H2,1-2H3
InchiKey:	OELHQHILWOIUSL-UHFFFAOYSA-N
Formula:	C8H17Br
SMILES:	CCCCC(Br)CC
Mol. weight [g/mol]:	193.12
CAS:	999-64-4

Physical Properties

Property code	Value	Unit	Source
gf	28.36	kJ/mol	Joback Method
hf	-187.40	kJ/mol	Joback Method
hfus	18.24	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.740		Crippen Method
mcvol	141.080	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
tb	448.16	K	Joback Method
tc	633.14	K	Joback Method
tf	224.72	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.18	J/mol×K	448.16	Joback Method
cpg	290.54	J/mol×K	478.99	Joback Method
cpg	303.29	J/mol×K	509.82	Joback Method
cpg	315.46	J/mol×K	540.65	Joback Method
cpg	327.07	J/mol×K	571.48	Joback Method
cpg	338.14	J/mol×K	602.31	Joback Method

cpg	348.69	J/mol×K	633.14	Joback Method
dvisc	0.0063866	Pa×s	224.72	Joback Method
dvisc	0.0026570	Pa×s	261.96	Joback Method
dvisc	0.0013751	Pa×s	299.20	Joback Method
dvisc	0.0008234	Pa×s	336.44	Joback Method
dvisc	0.0005461	Pa×s	373.68	Joback Method
dvisc	0.0003902	Pa×s	410.92	Joback Method
dvisc	0.0002948	Pa×s	448.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50922e+01
Coeff. B	-4.14278e+03
Coeff. C	-6.94890e+01
Temperature range (K), min.	349.32
Temperature range (K), max.	493.06

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=C999644&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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