1-Bromo-6-methyloctane

Inchi: InChI=1S/C9H19Br/c1-3-9(2)7-5-4-6-8-10/h9H,3-8H2,1-2H3
InchiKey: TWDAVWNDGHYAJZ-UHFFFAOYSA-N
Formula: C9H19Br
SMILES: CCC(C)CCCCCBr
Mol. weight [g/mol]: 207.15
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	36.78	kJ/mol	Joback Method
hf	-208.04	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	41.67	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.988		Crippen Method
mcvol	155.170	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1225.00		NIST Webbook
tb	471.04	K	Joback Method
tc	654.26	K	Joback Method
tf	235.99	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.17	J/mol×K	471.04	Joback Method
cpg	334.50	J/mol×K	501.58	Joback Method
cpg	348.18	J/mol×K	532.11	Joback Method
cpg	361.24	J/mol×K	562.65	Joback Method
cpg	373.71	J/mol×K	593.19	Joback Method
cpg	385.59	J/mol×K	623.72	Joback Method
cpg	396.92	J/mol×K	654.26	Joback Method
dvisc	0.0062321	Pa×s	235.99	Joback Method

dvisc	0.0025512	Pa×s	275.17	Joback Method
dvisc	0.0013048	Pa×s	314.34	Joback Method
dvisc	0.0007742	Pa×s	353.51	Joback Method
dvisc	0.0005098	Pa×s	392.69	Joback Method
dvisc	0.0003622	Pa×s	431.86	Joback Method
dvisc	0.0002723	Pa×s	471.04	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53267e+01
Coeff. B	-4.38820e+03
Coeff. C	-7.58550e+01
Temperature range (K), min.	367.64
Temperature range (K), max.	514.01

Sources

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
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=R412583&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
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