2-Bromo-6-methylheptane

Inchi: InChI=1S/C8H17Br/c1-7(2)5-4-6-8(3)9/h7-8H,4-6H2,1-3H3
InchiKey: ZMWRLWROCBQAMW-UHFFFAOYSA-N
Formula: C8H17Br
SMILES: CC(C)CCCC(C)Br
Mol. weight [g/mol]: 193.12
CAS: 4730-24-9

Physical Properties

Property code	Value	Unit	Source
gf	25.92	kJ/mol	Joback Method
hf	-192.68	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	39.06	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.596		Crippen Method
mcvol	141.080	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
tb	447.72	K	Joback Method
tc	636.90	K	Joback Method
tf	209.72	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.27	J/mol×K	447.72	Joback Method
cpg	291.02	J/mol×K	479.25	Joback Method
cpg	304.12	J/mol×K	510.78	Joback Method
cpg	316.61	J/mol×K	542.31	Joback Method
cpg	328.51	J/mol×K	573.84	Joback Method
cpg	339.83	J/mol×K	605.37	Joback Method
cpg	350.60	J/mol×K	636.90	Joback Method
dvisc	0.0103997	Pa×s	209.72	Joback Method
dvisc	0.0035313	Pa×s	249.39	Joback Method

dvisc	0.0016129	Pa×s	289.05	Joback Method
dvisc	0.0008900	Pa×s	328.72	Joback Method
dvisc	0.0005582	Pa×s	368.39	Joback Method
dvisc	0.0003833	Pa×s	408.05	Joback Method
dvisc	0.0002814	Pa×s	447.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44199e+01
Coeff. B	-3.89786e+03
Coeff. C	-6.73480e+01
Temperature range (K), min.	343.16
Temperature range (K), max.	495.29

Sources

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=C4730249&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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