5-Bromo-1-hexene

Inchi: InChI=1S/C6H11Br/c1-3-4-5-6(2)7/h3,6H,1,4-5H2,2H3
InchiKey: AIAXFFLNNULCFG-UHFFFAOYSA-N
Formula: C6H11Br
SMILES: C=CCCC(C)Br
Mol. weight [g/mol]: 163.06
CAS: 4558-27-4

Physical Properties

Property code	Value	Unit	Source
gf	99.36	kJ/mol	Joback Method
hf	-20.69	kJ/mol	Joback Method
hfus	11.78	kJ/mol	Joback Method
hvap	34.33	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.736		Crippen Method
mcvol	108.600	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	399.08	K	Joback Method
tc	591.31	K	Joback Method
tf	200.42	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.92	J/mol×K	399.08	Joback Method
cpg	229.66	J/mol×K	559.28	Joback Method
cpg	221.28	J/mol×K	527.24	Joback Method
cpg	212.43	J/mol×K	495.20	Joback Method
cpg	203.10	J/mol×K	463.16	Joback Method
cpg	193.27	J/mol×K	431.12	Joback Method
cpg	237.61	J/mol×K	591.31	Joback Method
dvisc	0.0003294	Pa×s	399.08	Joback Method
dvisc	0.0004258	Pa×s	365.97	Joback Method

dvisc	0.0005794	Pa×s	332.86	Joback Method
dvisc	0.0008438	Pa×s	299.75	Joback Method
dvisc	0.0013491	Pa×s	266.64	Joback Method
dvisc	0.0024640	Pa×s	233.53	Joback Method
dvisc	0.0054914	Pa×s	200.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59253e+01
Coeff. B	-4.01267e+03
Coeff. C	-5.71180e+01
Temperature range (K), min.	313.72
Temperature range (K), max.	435.18

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4558274&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

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

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

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