2-Bromo-2-methylhexane

Inchi: InChI=1S/C7H15Br/c1-4-5-6-7(2,3)8/h4-6H2,1-3H3
InchiKey: FVGJIAVGOPDNHY-UHFFFAOYSA-N
Formula: C7H15Br
SMILES: CCCCC(C)(C)Br
Mol. weight [g/mol]: 179.10
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.3876		Cheméo Relay (1.0)
gf	25.22	kJ/mol	Joback Method
hf	-181.86	kJ/mol	Cheméo Relay (1.0)
hfus	11.76	kJ/mol	Joback Method
hvap	42.59	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	3.350		Crippen Method
mcvol	126.990	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	942.00		NIST Webbook
rinpol	942.00		NIST Webbook
tb	419.21	K	Cheméo Relay (1.0)
tc	609.94	K	Cheméo Relay (1.0)
tf	186.97	K	Cheméo Relay (1.0)
vc	0.467	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.41	J/mol×K	422.49	Joback Method
cpg	251.68	J/mol×K	454.92	Joback Method
cpg	264.20	J/mol×K	487.35	Joback Method
cpg	276.00	J/mol×K	519.78	Joback Method
cpg	287.12	J/mol×K	552.21	Joback Method
cpg	297.60	J/mol×K	584.64	Joback Method

cpg	307.48	J/mol×K	617.07	Joback Method
dvisc	0.0065777	Pa×s	230.87	Joback Method
dvisc	0.0029947	Pa×s	262.81	Joback Method
dvisc	0.0016169	Pa×s	294.74	Joback Method
dvisc	0.0009848	Pa×s	326.68	Joback Method
dvisc	0.0006552	Pa×s	358.62	Joback Method
dvisc	0.0004659	Pa×s	390.55	Joback Method
dvisc	0.0003489	Pa×s	422.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43471e+01
Coeff. B	-3.71705e+03
Coeff. C	-6.12600e+01
Temperature range (K), min.	325.64
Temperature range (K), max.	472.64

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R32428&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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