

1-Heptene, 7-bromo

Other names:	bromo-7 heptene-1
Inchi:	InChI=1S/C7H13Br/c1-2-3-4-5-6-7-8/h2H,1,3-7H2
InchiKey:	GNYDYUQVALBGGZ-UHFFFAOYSA-N
Formula:	C7H13Br
SMILES:	C=CCCCCCBr
Mol. weight [g/mol]:	177.08

Physical Properties

Property code	Value	Unit	Source
gf	110.22	kJ/mol	Joback Method
hf	-36.05	kJ/mol	Joback Method
hfus	17.89	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.128		Crippen Method
mvol	122.690	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
ripol	1008.00		NIST Webbook
ripol	1358.00		NIST Webbook
tb	422.40	K	Joback Method
tc	608.68	K	Joback Method
tf	226.69	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.71	J/mol×K	422.40	Joback Method
cpg	231.97	J/mol×K	453.45	Joback Method
cpg	242.69	J/mol×K	484.49	Joback Method
cpg	252.89	J/mol×K	515.54	Joback Method
cpg	262.59	J/mol×K	546.59	Joback Method
cpg	271.80	J/mol×K	577.64	Joback Method
cpg	280.56	J/mol×K	608.68	Joback Method

dvisc	0.0037219	Paxs	226.69	Joback Method
dvisc	0.0019239	Paxs	259.31	Joback Method
dvisc	0.0011525	Paxs	291.93	Joback Method
dvisc	0.0007653	Paxs	324.54	Joback Method
dvisc	0.0005477	Paxs	357.16	Joback Method
dvisc	0.0004145	Paxs	389.78	Joback Method
dvisc	0.0003275	Paxs	422.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R133854&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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