

Hexane, 2-bromo-1-methoxy

Inchi:	InChI=1S/C7H15BrO/c1-3-4-5-7(8)6-9-2/h7H,3-6H2,1-2H3
InchiKey:	NKEKBMXDTJGVMN-UHFFFAOYSA-N
Formula:	C7H15BrO
SMILES:	CCCCC(Br)COC
Mol. weight [g/mol]:	195.10

Physical Properties

Property code	Value	Unit	Source
gf	-85.06	kJ/mol	Joback Method
hf	-298.98	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.587		Crippen Method
mcvol	132.860	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpola	1028.00		NIST Webbook
tb	447.70	K	Joback Method
tc	633.73	K	Joback Method
tf	235.68	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.73	J/molxK	447.70	Joback Method
cpg	271.68	J/molxK	478.71	Joback Method
cpg	283.16	J/molxK	509.71	Joback Method
cpg	294.17	J/molxK	540.72	Joback Method
cpg	304.72	J/molxK	571.72	Joback Method
cpg	314.83	J/molxK	602.73	Joback Method
cpg	324.49	J/molxK	633.73	Joback Method
dvisc	0.0045222	Paxs	235.68	Joback Method
dvisc	0.0020680	Paxs	271.02	Joback Method

dvisc	0.0011328	Paxs	306.35	Joback Method
dvisc	0.0007028	Paxs	341.69	Joback Method
dvisc	0.0004768	Paxs	377.03	Joback Method
dvisc	0.0003457	Paxs	412.36	Joback Method
dvisc	0.0002637	Paxs	447.70	Joback Method

Sources

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=R12010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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