

1-Heptanol, 7-bromo-

Inchi:	InChI=1S/C7H15BrO/c8-6-4-2-1-3-5-7-9/h9H,1-7H2
InchiKey:	MMXRNUXCHUHOE-UHFFFAOYSA-N
Formula:	C7H15BrO
SMILES:	OCCCCCBr
Mol. weight [g/mol]:	195.10
CAS:	10160-24-4

Physical Properties

Property code	Value	Unit	Source
gf	-114.44	kJ/mol	Joback Method
hf	-313.71	kJ/mol	Joback Method
hfus	23.26	kJ/mol	Joback Method
hvap	54.29	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.324		Crippen Method
mcvol	132.860	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	517.90	K	Joback Method
tc	692.62	K	Joback Method
tf	289.27	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.83	J/molxK	517.90	Joback Method
cpg	333.56	J/molxK	663.50	Joback Method
cpg	325.06	J/molxK	634.38	Joback Method
cpg	316.15	J/molxK	605.26	Joback Method
cpg	306.82	J/molxK	576.14	Joback Method
cpg	297.05	J/molxK	547.02	Joback Method
cpg	341.68	J/molxK	692.62	Joback Method
dvisc	0.0001709	Paxs	517.90	Joback Method
dvisc	0.0002697	Paxs	479.79	Joback Method

dvisc	0.0004604	Paxs	441.69	Joback Method
dvisc	0.0008694	Paxs	403.58	Joback Method
dvisc	0.0018745	Paxs	365.48	Joback Method
dvisc	0.0048329	Paxs	327.38	Joback Method
dvisc	0.0159918	Paxs	289.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.70	K	0.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10160244&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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