

1-Nonanol, 9-bromo-

Other names:	9-Bromo-1-nonanol
Inchi:	InChI=1S/C9H19BrO/c10-8-6-4-2-1-3-5-7-9-11/h11H,1-9H2
InchiKey:	USJDOLXCPFASNV-UHFFFAOYSA-N
Formula:	C9H19BrO
SMILES:	OCCCCCCCCCBr
Mol. weight [g/mol]:	223.15
CAS:	55362-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-97.60	kJ/mol	Joback Method
hf	-354.99	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	58.74	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.104		Crippen Method
mcvol	161.040	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	563.66	K	Joback Method
tc	735.67	K	Joback Method
tf	311.81	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.66	J/molxK	563.66	Joback Method
cpg	389.56	J/molxK	592.33	Joback Method
cpg	400.93	J/molxK	621.00	Joback Method
cpg	411.80	J/molxK	649.67	Joback Method
cpg	422.18	J/molxK	678.34	Joback Method
cpg	432.10	J/molxK	707.01	Joback Method
cpg	441.57	J/molxK	735.67	Joback Method
dvisc	0.0106889	Paxs	311.81	Joback Method

dvisc	0.0032090	Paxs	353.78	Joback Method
dvisc	0.0012435	Paxs	395.76	Joback Method
dvisc	0.0005780	Paxs	437.74	Joback Method
dvisc	0.0003072	Paxs	479.71	Joback Method
dvisc	0.0001807	Paxs	521.68	Joback Method
dvisc	0.0001151	Paxs	563.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	0.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55362806&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
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
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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