1-Undecanol, 11-bromo-

Other names: 1-Bromo-11-hydroxyundecane
11-Bromo-1-hydroxyundecane
11-Bromoundecanol
11-Bromoundecan-1-ol
11-Bromo-1-undecanol
Inchi: InChI=1S/C11H23BrO/c12-10-8-6-4-2-1-3-5-7-9-11-13/h13H,1-11H2
InchiKey: XFGANBYCJWQYBI-UHFFFAOYSA-N
Formula: C11H23BrO
SMILES: OCCCCCCCCCCCBr
Mol. weight [g/mol]: 251.20
CAS: 1611-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-80.76	kJ/mol	Joback Method
hf	-396.27	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	63.19	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.885		Crippen Method
mcvol	189.220	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
tb	609.42	K	Joback Method
tc	779.55	K	Joback Method
tf	334.35	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.35	J/mol×K	609.42	Joback Method
cpg	488.63	J/mol×K	637.77	Joback Method
cpg	501.32	J/mol×K	666.13	Joback Method
cpg	513.45	J/mol×K	694.48	Joback Method

cpg	525.05	J/mol×K	722.84	Joback Method
cpg	536.12	J/mol×K	751.19	Joback Method
cpg	546.70	J/mol×K	779.55	Joback Method
dvisc	0.0071648	Pa×s	334.35	Joback Method
dvisc	0.0021400	Pa×s	380.19	Joback Method
dvisc	0.0008290	Pa×s	426.04	Joback Method
dvisc	0.0003861	Pa×s	471.88	Joback Method
dvisc	0.0002059	Pa×s	517.73	Joback Method
dvisc	0.0001216	Pa×s	563.58	Joback Method
dvisc	0.0000778	Pa×s	609.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.70	K	0.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1611569&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