8-BROMO-1-OCTANOL

Other names: 1-Octanol, 8-bromo-
8-bromooctan-1-ol
Inchi: InChI=1S/C8H17BrO/c9-7-5-3-1-2-4-6-8-10/h10H,1-8H2
InchiKey: GMXIEASXPUEOTG-UHFFFAOYSA-N
Formula: C8H17BrO
SMILES: OCCCCCCCCBr
Mol. weight [g/mol]: 209.13

Physical Properties

Property code	Value	Unit	Source
af	0.7913		Cheméo Relay (1.0)
gf	-106.02	kJ/mol	Joback Method
hf	-359.71	kJ/mol	Cheméo Relay (1.0)
hfus	25.85	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
log10ws	-2.92		Cheméo Relay (1.0)
logp	2.714		Crippen Method
mcvol	146.950	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	541.95	K	Cheméo Relay (1.0)
tc	738.63	K	Cheméo Relay (1.0)
tf	285.99	K	Cheméo Relay (1.0)
vc	0.544	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.34	J/mol×K	540.78	Joback Method
cpg	342.44	J/mol×K	569.66	Joback Method
cpg	353.05	J/mol×K	598.54	Joback Method
cpg	363.19	J/mol×K	627.43	Joback Method
cpg	372.87	J/mol×K	656.31	Joback Method
cpg	382.12	J/mol×K	685.19	Joback Method

cpg	390.95	J/mol×K	714.07	Joback Method
dvisc	0.0130696	Pa×s	300.54	Joback Method
dvisc	0.0039358	Pa×s	340.58	Joback Method
dvisc	0.0015257	Pa×s	380.62	Joback Method
dvisc	0.0007084	Pa×s	420.66	Joback Method
dvisc	0.0003758	Pa×s	460.70	Joback Method
dvisc	0.0002206	Pa×s	500.74	Joback Method
dvisc	0.0001402	Pa×s	540.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50816198&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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