1-Bromo-8-tetrahydropyranyloxyoctane

Other names: 2H-Pyran, 2-[(8-bromooctyl)oxy]tetrahydro-
8-Bromooctyl tetrahydropyranyl ether
2-[(8-bromooctyl)oxy]tetrahydro-2H-pyran
Inchi: InChI=1S/C13H25BrO2/c14-10-6-3-1-2-4-7-11-15-13-9-5-8-12-16-13/h13H,1-12H2
InchiKey: JCRBYQZIJFWGOO-UHFFFAOYSA-N
Formula: C13H25BrO2
SMILES: BrCCCCCCCCOC1CCCCO1
Mol. weight [g/mol]: 293.24
CAS: 50816-20-1

Physical Properties

Property code	Value	Unit	Source
gf	-93.77	kJ/mol	Joback Method
hf	-495.22	kJ/mol	Joback Method
hfus	35.71	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.265		Crippen Method
mcvol	212.410	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	631.92	K	Joback Method
tc	831.92	K	Joback Method
tf	352.25	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.10	J/mol×K	631.92	Joback Method
cpg	585.00	J/mol×K	665.25	Joback Method
cpg	602.86	J/mol×K	698.59	Joback Method
cpg	619.72	J/mol×K	731.92	Joback Method
cpg	635.61	J/mol×K	765.26	Joback Method
cpg	650.54	J/mol×K	798.59	Joback Method

cpg	664.56	J/mol×K	831.92	Joback Method
dvisc	0.0026778	Pa×s	352.25	Joback Method
dvisc	0.0012516	Pa×s	398.86	Joback Method
dvisc	0.0006859	Pa×s	445.47	Joback Method
dvisc	0.0004213	Pa×s	492.08	Joback Method
dvisc	0.0002815	Pa×s	538.70	Joback Method
dvisc	0.0002006	Pa×s	585.31	Joback Method
dvisc	0.0001503	Pa×s	631.92	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50816201&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume