p-Bromophenyl octyl ether

Inchi: InChI=1S/C14H21BrO/c1-2-3-4-5-6-7-12-16-14-10-8-13(15)9-11-14/h8-11H,2-7,12H2,1H
InchiKey: UVBFFPZGOOKWNR-UHFFFAOYSA-N
Formula: C14H21BrO
SMILES: CCCCCCCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 285.22
CAS: 96693-05-9

Physical Properties

Property code	Value	Unit	Source
gf	79.10	kJ/mol	Joback Method
hf	-213.12	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.188		Crippen Method
mcvol	207.730	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
tb	639.96	K	Joback Method
tc	845.42	K	Joback Method
tf	368.51	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.46	J/mol×K	639.96	Joback Method
cpg	533.74	J/mol×K	674.20	Joback Method
cpg	549.10	J/mol×K	708.45	Joback Method
cpg	563.58	J/mol×K	742.69	Joback Method
cpg	577.22	J/mol×K	776.93	Joback Method
cpg	590.04	J/mol×K	811.17	Joback Method
cpg	602.09	J/mol×K	845.42	Joback Method
dvisc	0.0013694	Pa×s	368.51	Joback Method
dvisc	0.0007525	Pa×s	413.75	Joback Method

dvisc	0.0004653	Pa×s	458.99	Joback Method
dvisc	0.0003137	Pa×s	504.24	Joback Method
dvisc	0.0002256	Pa×s	549.48	Joback Method
dvisc	0.0001706	Pa×s	594.72	Joback Method
dvisc	0.0001342	Pa×s	639.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	409.00 ± 1.00	K	0.07	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96693059&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