

p-Bromophenyoctane

Other names:	p-Octylbromobenzene
Inchi:	InChI=1S/C14H21Br/c1-2-3-4-5-6-7-8-13-9-11-14(15)12-10-13/h9-12H,2-8H2,1H3
InchiKey:	OOZQSVXPBCINJF-UHFFFAOYSA-N
Formula:	C14H21Br
SMILES:	CCCCCCCCc1ccc(Br)cc1
Mol. weight [g/mol]:	269.22
CAS:	51554-93-9

Physical Properties

Property code	Value	Unit	Source
gf	184.10	kJ/mol	Joback Method
hf	-80.90	kJ/mol	Joback Method
hfus	30.95	kJ/mol	Joback Method
hvap	56.13	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.352		Crippen Method
mcvol	201.860	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
tb	617.54	K	Joback Method
tc	825.06	K	Joback Method
tf	346.28	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.40	J/molxK	617.54	Joback Method
cpg	507.06	J/molxK	652.13	Joback Method
cpg	522.75	J/molxK	686.71	Joback Method
cpg	537.54	J/molxK	721.30	Joback Method
cpg	551.46	J/molxK	755.89	Joback Method
cpg	564.55	J/molxK	790.48	Joback Method
cpg	576.88	J/molxK	825.06	Joback Method
dvisc	0.0018994	Paxs	346.28	Joback Method

dvisc	0.0010094	Paxs	391.49	Joback Method
dvisc	0.0006115	Paxs	436.70	Joback Method
dvisc	0.0004069	Paxs	481.91	Joback Method
dvisc	0.0002904	Paxs	527.12	Joback Method
dvisc	0.0002186	Paxs	572.33	Joback Method
dvisc	0.0001715	Paxs	617.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.50 ± 1.50	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=C51554939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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