

p-Bromophenyl butyl ether

Inchi:	InChI=1S/C10H13BrO/c1-2-3-8-12-10-6-4-9(11)5-7-10/h4-7H,2-3,8H2,1H3
InchiKey:	BOUVKHWPQNEXTO-UHFFFAOYSA-N
Formula:	C10H13BrO
SMILES:	CCCCOc1ccc(Br)cc1
Mol. weight [g/mol]:	229.11
CAS:	39969-57-8

Physical Properties

Property code	Value	Unit	Source
gf	45.42	kJ/mol	Joback Method
hf	-130.56	kJ/mol	Joback Method
hfus	21.78	kJ/mol	Joback Method
hvap	49.64	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.628		Crippen Method
mcvol	151.370	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	548.44	K	Joback Method
tc	767.82	K	Joback Method
tf	323.43	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.07	J/molxK	548.44	Joback Method
cpg	335.63	J/molxK	585.00	Joback Method
cpg	348.41	J/molxK	621.57	Joback Method
cpg	360.44	J/molxK	658.13	Joback Method
cpg	371.74	J/molxK	694.70	Joback Method
cpg	382.35	J/molxK	731.26	Joback Method
cpg	392.28	J/molxK	767.82	Joback Method
dvisc	0.0016322	Paxs	323.43	Joback Method
dvisc	0.0009634	Paxs	360.93	Joback Method

dvisc	0.0006280	Paxs	398.43	Joback Method
dvisc	0.0004406	Paxs	435.94	Joback Method
dvisc	0.0003270	Paxs	473.44	Joback Method
dvisc	0.0002536	Paxs	510.94	Joback Method
dvisc	0.0002036	Paxs	548.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.50 ± 1.50	K	6.70	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39969578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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