

P-hexyloxybromobenzene

Inchi:	InChI=1S/C12H17BrO/c1-2-3-4-5-10-14-12-8-6-11(13)7-9-12/h6-9H,2-5,10H2,1H3
InchiKey:	GKLMJONYGGTHHM-UHFFFAOYSA-N
Formula:	C12H17BrO
SMILES:	CCCCCOc1ccc(Br)cc1
Mol. weight [g/mol]:	257.17
CAS:	30752-19-3

Physical Properties

Property code	Value	Unit	Source
gf	62.26	kJ/mol	Joback Method
hf	-171.84	kJ/mol	Joback Method
hfus	26.96	kJ/mol	Joback Method
hvap	54.09	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.408		Crippen Method
mvol	179.550	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
tb	594.20	K	Joback Method
tc	806.18	K	Joback Method
tf	345.97	K	Joback Method
vc	0.679	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.58	J/molxK	594.20	Joback Method
cpg	431.71	J/molxK	629.53	Joback Method
cpg	445.98	J/molxK	664.86	Joback Method
cpg	459.43	J/molxK	700.19	Joback Method
cpg	472.08	J/molxK	735.52	Joback Method
cpg	483.96	J/molxK	770.85	Joback Method
cpg	495.11	J/molxK	806.18	Joback Method
dvisc	0.0015238	Paxs	345.97	Joback Method
dvisc	0.0008663	Paxs	387.34	Joback Method

dvisc	0.0005492	Paxs	428.71	Joback Method
dvisc	0.0003772	Paxs	470.09	Joback Method
dvisc	0.0002754	Paxs	511.46	Joback Method
dvisc	0.0002107	Paxs	552.83	Joback Method
dvisc	0.0001673	Paxs	594.20	Joback Method

Sources

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=C30752193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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