2-Bromobenzyl alcohol, n-pentyl ether

Inchi: InChI=1S/C12H17BrO/c1-2-3-6-9-14-10-11-7-4-5-8-12(11)13/h4-5,7-8H,2-3,6,9-10H2,1H
InchiKey: WJWANQRTZJQLOE-UHFFFAOYSA-N
Formula: C12H17BrO
SMILES: CCCCCOCc1ccccc1Br
Mol. weight [g/mol]: 257.17

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	-4.69		Crippen Method
logp	4.156		Crippen Method
mcvol	179.550	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1632.00		NIST Webbook
tb	594.20	K	Joback Method
tc	806.18	K	Joback Method
tf	345.97	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.58	J/mol×K	594.20	Joback Method
cpg	483.96	J/mol×K	770.85	Joback Method
cpg	472.08	J/mol×K	735.52	Joback Method
cpg	459.43	J/mol×K	700.19	Joback Method
cpg	445.98	J/mol×K	664.86	Joback Method
cpg	431.71	J/mol×K	629.53	Joback Method
cpg	495.11	J/mol×K	806.18	Joback Method
dvisc	0.0001673	Pa×s	594.20	Joback Method
dvisc	0.0002107	Pa×s	552.83	Joback Method

dvisc	0.0002754	Pa×s	511.46	Joback Method
dvisc	0.0003772	Pa×s	470.09	Joback Method
dvisc	0.0005492	Pa×s	428.71	Joback Method
dvisc	0.0008663	Pa×s	387.34	Joback Method
dvisc	0.0015238	Pa×s	345.97	Joback Method

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=U378188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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