4-Bromobutyric acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C17H17BrO3/c18-12-4-7-17(19)21-16-10-8-15(9-11-16)20-13-14-5-2-1-3-6-14/
InchiKey: NDYIZAFRVHKCHC-UHFFFAOYSA-N
Formula: C17H17BrO3
SMILES: O=C(CCCBr)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 349.22

Physical Properties

Property code	Value	Unit	Source
gf	-17.15	kJ/mol	Joback Method
hf	-283.31	kJ/mol	Joback Method
hfus	36.74	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.346		Crippen Method
mcvol	233.680	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2568.00		NIST Webbook
rinpol	2568.00		NIST Webbook
tb	811.57	K	Joback Method
tc	1047.65	K	Joback Method
tf	500.90	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.62	J/mol×K	811.57	Joback Method
cpg	693.25	J/mol×K	1008.30	Joback Method
cpg	683.94	J/mol×K	968.96	Joback Method
cpg	673.57	J/mol×K	929.61	Joback Method
cpg	662.09	J/mol×K	890.26	Joback Method
cpg	649.46	J/mol×K	850.92	Joback Method
cpg	701.56	J/mol×K	1047.65	Joback Method
dvisc	0.0000708	Pa×s	811.57	Joback Method

dvisc	0.0000889	Pa×s	759.79	Joback Method
dvisc	0.0001153	Pa×s	708.01	Joback Method
dvisc	0.0001558	Pa×s	656.24	Joback Method
dvisc	0.0002217	Pa×s	604.46	Joback Method
dvisc	0.0003370	Pa×s	552.68	Joback Method
dvisc	0.0005585	Pa×s	500.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307614&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume