5-Bromovaleric acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C18H19BrO3/c19-13-5-4-8-18(20)22-17-11-9-16(10-12-17)21-14-15-6-2-1-3-7-
InchiKey: GNHFCKXWBUOWRM-UHFFFAOYSA-N
Formula: C18H19BrO3
SMILES: O=C(CCCCBr)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 363.25

Physical Properties

Property code	Value	Unit	Source
gf	-8.73	kJ/mol	Joback Method
hf	-303.95	kJ/mol	Joback Method
hfus	39.33	kJ/mol	Joback Method
hvap	78.88	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.736		Crippen Method
mcvol	247.770	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook
tb	834.45	K	Joback Method
tc	1066.99	K	Joback Method
tf	512.17	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.21	J/mol×K	834.45	Joback Method
cpg	705.25	J/mol×K	873.21	Joback Method
cpg	718.07	J/mol×K	911.96	Joback Method
cpg	729.73	J/mol×K	950.72	Joback Method
cpg	740.28	J/mol×K	989.48	Joback Method
cpg	749.78	J/mol×K	1028.23	Joback Method
cpg	758.27	J/mol×K	1066.99	Joback Method
dvisc	0.0005082	Pa×s	512.17	Joback Method

dvisc	0.0003027	Pa×s	565.88	Joback Method
dvisc	0.0001972	Pa×s	619.60	Joback Method
dvisc	0.0001376	Pa×s	673.31	Joback Method
dvisc	0.0001012	Pa×s	727.02	Joback Method
dvisc	0.0000777	Pa×s	780.74	Joback Method
dvisc	0.0000617	Pa×s	834.45	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=U307649&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