5-Chlorovaleric acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C18H19ClO3/c19-13-5-4-8-18(20)22-17-11-9-16(10-12-17)21-14-15-6-2-1-3-7-

InchiKey: WXPUTBOXHOZGMQ-UHFFFAOYSA-N

Formula: C18H19ClO3

SMILES: O=C(CCCCCl)Oc1ccc(OCc2ccccc2)cc1

Mol. weight [g/mol]: 318.80

Physical Properties

Property code	Value	Unit	Source
gf	-34.98	kJ/mol	Joback Method
hf	-346.02	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	76.83	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.580		Crippen Method
mcvol	242.510	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	805.72	K	Joback Method
tc	1031.64	K	Joback Method
tf	482.29	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.38	J/mol×K	805.72	Joback Method
cpg	740.67	J/mol×K	993.99	Joback Method
cpg	730.69	J/mol×K	956.33	Joback Method
cpg	719.61	J/mol×K	918.68	Joback Method
cpg	707.39	J/mol×K	881.03	Joback Method
cpg	693.99	J/mol×K	843.37	Joback Method
cpg	749.59	J/mol×K	1031.64	Joback Method
dvisc	0.0000663	Pa×s	805.72	Joback Method

dvisc	0.0000842	Pa×s	751.82	Joback Method
dvisc	0.0001109	Pa×s	697.91	Joback Method
dvisc	0.0001530	Pa×s	644.00	Joback Method
dvisc	0.0002239	Pa×s	590.10	Joback Method
dvisc	0.0003536	Pa×s	536.20	Joback Method
dvisc	0.0006185	Pa×s	482.29	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307982&Units=SI

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