4-Benzyloxy-3-chlorophenylacetic acid

Other names: [3-chloro-4-(phenylmethoxy)phenyl]acetic acid
Inchi: InChI=1S/C15H13ClO3/c16-13-8-12(9-15(17)18)6-7-14(13)19-10-11-4-2-1-3-5-11/h1-8H,
InchiKey: DFHBBMJTBBLQSA-UHFFFAOYSA-N
Formula: C15H13ClO3
SMILES: O=C(O)Cc1ccc(OCc2ccccc2)c(Cl)c1
Mol. weight [g/mol]: 276.71
CAS: 60736-70-1

Physical Properties

Property code	Value	Unit	Source
gf	-101.69	kJ/mol	Joback Method
hf	-315.58	kJ/mol	Joback Method
hfus	32.98	kJ/mol	Joback Method
hvap	85.08	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.546		Crippen Method
mcvol	200.240	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	2207.00		NIST Webbook
rinpol	2207.00		NIST Webbook
tb	811.82	K	Joback Method
tc	1036.15	K	Joback Method
tf	499.59	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.58	J/mol×K	811.82	Joback Method
cpg	549.47	J/mol×K	849.21	Joback Method
cpg	559.45	J/mol×K	886.60	Joback Method
cpg	568.55	J/mol×K	923.98	Joback Method
cpg	576.82	J/mol×K	961.37	Joback Method
cpg	584.29	J/mol×K	998.76	Joback Method

cpg	591.00	J/mol×K	1036.15	Joback Method
dvisc	0.0004747	Pa×s	499.59	Joback Method
dvisc	0.0002253	Pa×s	551.63	Joback Method
dvisc	0.0001216	Pa×s	603.67	Joback Method
dvisc	0.0000724	Pa×s	655.70	Joback Method
dvisc	0.0000465	Pa×s	707.74	Joback Method
dvisc	0.0000317	Pa×s	759.78	Joback Method
dvisc	0.0000228	Pa×s	811.82	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=C60736701&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

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