

4-Chlorobenzyl benzoate

Inchi:	InChI=1S/C14H11ClO2/c15-13-8-6-11(7-9-13)10-17-14(16)12-4-2-1-3-5-12/h1-9H,10H2
InchiKey:	ARLTXMAKDGVKNK-UHFFFAOYSA-N
Formula:	C14H11ClO2
SMILES:	O=C(OCc1ccc(Cl)cc1)c1ccccc1
Mol. weight [g/mol]:	246.69
CAS:	20386-93-0

Physical Properties

Property code	Value	Unit	Source
gf	36.34	kJ/mol	Joback Method
hf	-131.24	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	65.51	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.697		Crippen Method
mcvol	180.280	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	691.78	K	Joback Method
tc	938.00	K	Joback Method
tf	414.98	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.76	J/mol×K	691.78	Joback Method
cpg	453.56	J/mol×K	732.82	Joback Method
cpg	466.19	J/mol×K	773.85	Joback Method
cpg	477.72	J/mol×K	814.89	Joback Method
cpg	488.18	J/mol×K	855.92	Joback Method
cpg	497.64	J/mol×K	896.96	Joback Method
cpg	506.14	J/mol×K	938.00	Joback Method
dvisc	0.0011566	Pa×s	414.98	Joback Method
dvisc	0.0006831	Pa×s	461.11	Joback Method

dvisc	0.0004441	Pa×s	507.25	Joback Method
dvisc	0.0003102	Pa×s	553.38	Joback Method
dvisc	0.0002289	Pa×s	599.51	Joback Method
dvisc	0.0001765	Pa×s	645.65	Joback Method
dvisc	0.0001408	Pa×s	691.78	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=C20386930&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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