4-butylbenzoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C14H17ClO2/c1-2-3-5-12-6-8-13(9-7-12)14(16)17-11-4-10-15/h4,6-10H,2-3,5,1
InchiKey: FDTZLBPFIUPWST-ONNFQVAWSA-N
Formula: C14H17ClO2
SMILES: CCCCc1ccc(C(=O)OC/C=C/Cl)cc1
Mol. weight [g/mol]: 252.74

Physical Properties

Property code	Value	Unit	Source
af	0.6519		Cheméo Relay (1.0)
hfus	32.85	kJ/mol	Joback Method
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-5.41		Cheméo Relay (1.0)
logp	3.939		Crippen Method
mcvol	199.740	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1930.40		NIST Webbook
tb	591.63	K	Cheméo Relay (1.0)
tc	786.38	K	Cheméo Relay (1.0)
tf	268.99	K	Cheméo Relay (1.0)
vc	0.699	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.61	J/mol×K	669.26	Joback Method
cpg	515.20	J/mol×K	704.67	Joback Method
cpg	528.88	J/mol×K	740.07	Joback Method
cpg	541.68	J/mol×K	775.48	Joback Method
cpg	553.66	J/mol×K	810.88	Joback Method
cpg	564.85	J/mol×K	846.29	Joback Method
cpg	575.29	J/mol×K	881.69	Joback Method
dvisc	0.0012851	Pa×s	383.48	Joback Method
dvisc	0.0006964	Pa×s	431.11	Joback Method
dvisc	0.0004263	Pa×s	478.74	Joback Method

dvisc	0.0002852	Pa×s	526.37	Joback Method
dvisc	0.0002040	Pa×s	574.00	Joback Method
dvisc	0.0001535	Pa×s	621.63	Joback Method
dvisc	0.0001204	Pa×s	669.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292529&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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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