Benzoic acid, 2-chloro, 1-methylpropyl ester

Other names: Benzoic acid, 2-chloro, 1-methylpropyl ester
Inchi: InChI=1S/C11H13ClO2/c1-3-8(2)14-11(13)9-6-4-5-7-10(9)12/h4-8H,3H2,1-2H3
InchiKey: PSVMSRFFQPHGTG-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: CCC(C)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 212.68

Physical Properties

Property code	Value	Unit	Source
hf	-401.73	kJ/mol	Cheméo Relay (1.0)
hfus	21.36	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-3.68		Cheméo Relay (1.0)
logp	3.295		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	2067.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2031.00		NIST Webbook
ripol	2054.00		NIST Webbook
tb	527.47	K	Cheméo Relay (1.0)
tf	254.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.26	J/mol×K	596.02	Joback Method
cpg	386.90	J/mol×K	632.51	Joback Method
cpg	399.73	J/mol×K	668.99	Joback Method
cpg	411.74	J/mol×K	705.48	Joback Method
cpg	422.97	J/mol×K	741.97	Joback Method
cpg	433.43	J/mol×K	778.45	Joback Method
cpg	443.15	J/mol×K	814.94	Joback Method
dvisc	0.0019955	Pa×s	339.75	Joback Method
dvisc	0.0010666	Pa×s	382.46	Joback Method
dvisc	0.0006465	Pa×s	425.17	Joback Method
dvisc	0.0004294	Pa×s	467.88	Joback Method
dvisc	0.0003054	Pa×s	510.60	Joback Method
dvisc	0.0002290	Pa×s	553.31	Joback Method
dvisc	0.0001789	Pa×s	596.02	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C97989281&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point