2-chlorobenzoic acid, undecyl ester

Other names: Benzoic acid, 2-chloro, undecyl ester
Inchi: InChI=1S/C18H27ClO2/c1-2-3-4-5-6-7-8-9-12-15-21-18(20)16-13-10-11-14-17(16)19/h10
InchiKey: LZZUEDTUAJZZBG-UHFFFAOYSA-N
Formula: C18H27ClO2
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 310.86

Physical Properties

Property code	Value	Unit	Source
af	0.8816		Cheméo Relay (1.0)
hf	-529.41	kJ/mol	Cheméo Relay (1.0)
hfus	43.01	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.63		Cheméo Relay (1.0)
logp	6.028		Crippen Method
mcvol	260.400	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2237.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2223.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2232.30		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2232.30		NIST Webbook
ripol	2841.00		NIST Webbook
ripol	2841.00		NIST Webbook
ripol	2897.00		NIST Webbook
ripol	2882.00		NIST Webbook
ripol	2861.00		NIST Webbook
ripol	2897.00		NIST Webbook
ripol	2880.00		NIST Webbook
ripol	2858.00		NIST Webbook
tb	613.30	K	Cheméo Relay (1.0)
tc	827.07	K	Cheméo Relay (1.0)

tf	284.63	K	Cheméo Relay (1.0)
vc	0.980	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.39	J/mol×K	756.62	Joback Method
cpg	757.96	J/mol×K	789.44	Joback Method
cpg	773.55	J/mol×K	822.26	Joback Method
cpg	788.18	J/mol×K	855.08	Joback Method
cpg	801.89	J/mol×K	887.90	Joback Method
cpg	814.71	J/mol×K	920.72	Joback Method
cpg	826.67	J/mol×K	953.54	Joback Method
dvisc	0.0010302	Pa×s	433.64	Joback Method
dvisc	0.0005413	Pa×s	487.47	Joback Method
dvisc	0.0003232	Pa×s	541.30	Joback Method
dvisc	0.0002119	Pa×s	595.13	Joback Method
dvisc	0.0001490	Pa×s	648.96	Joback Method
dvisc	0.0001106	Pa×s	702.79	Joback Method
dvisc	0.0000856	Pa×s	756.62	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97221960&Units=SI
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):

Legend

af: Acentric Factor
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume