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
CAS: 97221-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-42.39	kJ/mol	Joback Method
hf	-450.33	kJ/mol	Joback Method
hfus	43.01	kJ/mol	Joback Method
hvap	72.14	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.028		Crippen Method
mcvol	260.400	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2232.30		NIST Webbook
ripol	2841.00		NIST Webbook
ripol	2897.00		NIST Webbook
tb	756.62	K	Joback Method
tc	953.54	K	Joback Method
tf	433.64	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.39	J/mol×K	756.62	Joback Method
cpg	814.71	J/mol×K	920.72	Joback Method
cpg	801.89	J/mol×K	887.90	Joback Method

cpg	788.18	J/mol×K	855.08	Joback Method
cpg	773.55	J/mol×K	822.26	Joback Method
cpg	757.96	J/mol×K	789.44	Joback Method
cpg	826.67	J/mol×K	953.54	Joback Method
dvisc	0.0000856	Pa×s	756.62	Joback Method
dvisc	0.0001106	Pa×s	702.79	Joback Method
dvisc	0.0001490	Pa×s	648.96	Joback Method
dvisc	0.0002119	Pa×s	595.13	Joback Method
dvisc	0.0003232	Pa×s	541.30	Joback Method
dvisc	0.0005413	Pa×s	487.47	Joback Method
dvisc	0.0010302	Pa×s	433.64	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=C97221960&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume