Benzoic acid, 2-chloro, dodecyl ester

Inchi: InChI=1S/C19H29ClO2/c1-2-3-4-5-6-7-8-9-10-13-16-22-19(21)17-14-11-12-15-18(17)20/
InchiKey: CFPNNDJTTWZQME-UHFFFAOYSA-N
Formula: C19H29ClO2
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 324.88

Physical Properties

Property code	Value	Unit	Source
gf	-33.97	kJ/mol	Joback Method
hf	-470.97	kJ/mol	Joback Method
hfus	45.60	kJ/mol	Joback Method
hvap	74.37	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.418		Crippen Method
mcvol	274.490	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2313.00		NIST Webbook
ripol	3002.00		NIST Webbook
ripol	2943.00		NIST Webbook
tb	779.50	K	Joback Method
tc	975.71	K	Joback Method
tf	444.91	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.77	J/mol×K	779.50	Joback Method
cpg	815.62	J/mol×K	812.20	Joback Method
cpg	831.45	J/mol×K	844.90	Joback Method
cpg	846.30	J/mol×K	877.61	Joback Method
cpg	860.21	J/mol×K	910.31	Joback Method
cpg	873.21	J/mol×K	943.01	Joback Method

cpg	885.33	J/mol×K	975.71	Joback Method
dvisc	0.0009407	Pa×s	444.91	Joback Method
dvisc	0.0004880	Pa×s	500.68	Joback Method
dvisc	0.0002888	Pa×s	556.44	Joback Method
dvisc	0.0001880	Pa×s	612.20	Joback Method
dvisc	0.0001315	Pa×s	667.97	Joback Method
dvisc	0.0000972	Pa×s	723.73	Joback Method
dvisc	0.0000750	Pa×s	779.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R31373&Units=SI
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

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