Dodecyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, dodecyl ester
Inchi: InChI=1S/C19H29ClO2/c1-2-3-4-5-6-7-8-9-10-11-15-22-19(21)17-13-12-14-18(20)16-17/
InchiKey: MSKZMSLGYPWWRP-UHFFFAOYSA-N
Formula: C19H29ClO2
SMILES: CCCCCCCCCCCCOC(=O)c1cccc(Cl)c1
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	2317.00		NIST Webbook
rinpol	2394.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2334.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2394.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
ripol	2854.00		NIST Webbook
ripol	2854.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2898.00		NIST Webbook
ripol	2875.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2893.00		NIST Webbook
ripol	2870.00		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

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=U373568&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