2-Chlorobenzoic acid, 3-tetradecyl ester

Inchi: InChI=1S/C21H33ClO2/c1-3-5-6-7-8-9-10-11-12-15-18(4-2)24-21(23)19-16-13-14-17-20(
InchiKey: XVAHMORCDPFYJM-UHFFFAOYSA-N
Formula: C21H33ClO2
SMILES: CCCCCCCCCCCC(CC)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 352.94

Physical Properties

Property code	Value	Unit	Source
gf	-19.57	kJ/mol	Joback Method
hf	-517.53	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.196		Crippen Method
mcvol	302.670	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2419.00		NIST Webbook
tb	824.82	K	Joback Method
tc	1023.18	K	Joback Method
tf	452.45	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.82	J/mol×K	824.82	Joback Method
cpg	934.32	J/mol×K	857.88	Joback Method
cpg	950.71	J/mol×K	890.94	Joback Method
cpg	966.05	J/mol×K	924.00	Joback Method
cpg	980.36	J/mol×K	957.06	Joback Method
cpg	993.70	J/mol×K	990.12	Joback Method
cpg	1006.09	J/mol×K	1023.18	Joback Method
dvisc	0.0008970	Pa×s	452.45	Joback Method
dvisc	0.0004199	Pa×s	514.51	Joback Method

dvisc	0.0002314	Pa×s	576.57	Joback Method
dvisc	0.0001432	Pa×s	638.63	Joback Method
dvisc	0.0000965	Pa×s	700.70	Joback Method
dvisc	0.0000693	Pa×s	762.76	Joback Method
dvisc	0.0000523	Pa×s	824.82	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=U299818&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume