2-Chlorobenzoic acid, octadecyl ester

Inchi: InChI=1S/C25H41ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-28-25(27)23-20-
InchiKey: BVHRECHWYGIHRJ-UHFFFAOYSA-N
Formula: C25H41ClO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 409.05
CAS: 70153-10-5

Physical Properties

Property code	Value	Unit	Source
gf	16.55	kJ/mol	Joback Method
hf	-594.81	kJ/mol	Joback Method
hfus	61.14	kJ/mol	Joback Method
hvap	87.72	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.758		Crippen Method
mcvol	359.030	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	2996.70		NIST Webbook
rinpol	2996.70		NIST Webbook
tb	916.78	K	Joback Method
tc	1122.97	K	Joback Method
tf	512.53	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.65	J/mol×K	916.78	Joback Method
cpg	1241.25	J/mol×K	1088.60	Joback Method
cpg	1227.40	J/mol×K	1054.24	Joback Method
cpg	1212.48	J/mol×K	1019.87	Joback Method
cpg	1196.41	J/mol×K	985.51	Joback Method
cpg	1179.15	J/mol×K	951.14	Joback Method
cpg	1254.08	J/mol×K	1122.97	Joback Method

dvisc	0.0000320	Pa×s	916.78	Joback Method
dvisc	0.0000422	Pa×s	849.40	Joback Method
dvisc	0.0000583	Pa×s	782.03	Joback Method
dvisc	0.0000856	Pa×s	714.65	Joback Method
dvisc	0.0001362	Pa×s	647.28	Joback Method
dvisc	0.0002412	Pa×s	579.90	Joback Method
dvisc	0.0004967	Pa×s	512.53	Joback Method

Sources

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=C70153105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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