2-Chlorobenzoic acid, pentadecyl ester

Inchi: InChI=1S/C22H35ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-25-22(24)20-17-14-15-18-
InchiKey: KHLHBSPALROSMG-UHFFFAOYSA-N
Formula: C22H35ClO2
SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 366.96

Physical Properties

Property code	Value	Unit	Source
gf	-8.71	kJ/mol	Joback Method
hf	-532.89	kJ/mol	Joback Method
hfus	53.37	kJ/mol	Joback Method
hvap	81.05	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.588		Crippen Method
mcvol	316.760	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	2688.40		NIST Webbook
tb	848.14	K	Joback Method
tc	1045.97	K	Joback Method
tf	478.72	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.34	J/mol×K	848.14	Joback Method
cpg	993.95	J/mol×K	881.11	Joback Method
cpg	1010.45	J/mol×K	914.08	Joback Method
cpg	1025.89	J/mol×K	947.06	Joback Method
cpg	1040.30	J/mol×K	980.03	Joback Method
cpg	1053.74	J/mol×K	1013.00	Joback Method
cpg	1066.24	J/mol×K	1045.97	Joback Method
dvisc	0.0006960	Pa×s	478.72	Joback Method
dvisc	0.0003487	Pa×s	540.29	Joback Method

dvisc	0.0002012	Pa×s	601.86	Joback Method
dvisc	0.0001286	Pa×s	663.43	Joback Method
dvisc	0.0000887	Pa×s	725.00	Joback Method
dvisc	0.0000648	Pa×s	786.57	Joback Method
dvisc	0.0000496	Pa×s	848.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292430&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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