4-Chlorobenzoic acid, 2-propylphenyl ester

Inchi: InChI=1S/C16H15ClO2/c1-2-5-12-6-3-4-7-15(12)19-16(18)13-8-10-14(17)11-9-13/h3-4,6
InchiKey: OGXMTXCERAZEAE-UHFFFAOYSA-N
Formula: C16H15ClO2
SMILES: CCCc1ccccc1OC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 274.74

Physical Properties

Property code	Value	Unit	Source
gf	43.55	kJ/mol	Joback Method
hf	-183.99	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	70.63	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.512		Crippen Method
mcvol	208.460	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	742.52	K	Joback Method
tc	979.58	K	Joback Method
tf	450.04	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.57	J/mol×K	742.52	Joback Method
cpg	557.06	J/mol×K	782.03	Joback Method
cpg	570.40	J/mol×K	821.54	Joback Method
cpg	582.62	J/mol×K	861.05	Joback Method
cpg	593.77	J/mol×K	900.56	Joback Method
cpg	603.91	J/mol×K	940.07	Joback Method
cpg	613.07	J/mol×K	979.58	Joback Method
dvisc	0.0008553	Pa×s	450.04	Joback Method

dvisc	0.0005167	Pa×s	498.79	Joback Method
dvisc	0.0003415	Pa×s	547.53	Joback Method
dvisc	0.0002415	Pa×s	596.28	Joback Method
dvisc	0.0001799	Pa×s	645.03	Joback Method
dvisc	0.0001397	Pa×s	693.77	Joback Method
dvisc	0.0001122	Pa×s	742.52	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=U354629&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