

2-Chlorobenzoic acid, 2-propylphenyl ester

Inchi:	InChI=1S/C16H15ClO2/c1-2-7-12-8-3-6-11-15(12)19-16(18)13-9-4-5-10-14(13)17/h3-6,8
InchiKey:	VZKLYTCUIRNUIL-UHFFFAOYSA-N
Formula:	C16H15ClO2
SMILES:	CCc1ccccc1OC(=O)c1ccccc1Cl
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
rinpola	2089.00		NIST Webbook
tb	742.52	K	Joback Method
tc	979.58	K	Joback Method
tf	450.04	K	Joback Method
vc	0.788	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.57	J/molxK	742.52	Joback Method
cpg	603.91	J/molxK	940.07	Joback Method
cpg	593.77	J/molxK	900.56	Joback Method
cpg	582.62	J/molxK	861.05	Joback Method
cpg	570.40	J/molxK	821.54	Joback Method
cpg	557.06	J/molxK	782.03	Joback Method
cpg	613.07	J/molxK	979.58	Joback Method
dvisc	0.0001122	Paxs	742.52	Joback Method
dvisc	0.0001397	Paxs	693.77	Joback Method

dvisc	0.0001799	Paxs	645.03	Joback Method
dvisc	0.0002415	Paxs	596.28	Joback Method
dvisc	0.0003415	Paxs	547.53	Joback Method
dvisc	0.0005167	Paxs	498.79	Joback Method
dvisc	0.0008553	Paxs	450.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U360525&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

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