

2-Chlorobenzoic acid, 3-ethylphenyl ester

Inchi:	InChI=1S/C15H13ClO2/c1-2-11-6-5-7-12(10-11)18-15(17)13-8-3-4-9-14(13)16/h3-10H,2
InchiKey:	IYPBCYXCSGABDV-UHFFFAOYSA-N
Formula:	C15H13ClO2
SMILES:	CCc1cccc(OC(=O)c2ccccc2Cl)c1
Mol. weight [g/mol]:	260.72

Physical Properties

Property code	Value	Unit	Source
gf	35.13	kJ/mol	Joback Method
hf	-163.35	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	68.40	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.122		Crippen Method
mvol	194.370	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	2074.00		NIST Webbook
tb	719.64	K	Joback Method
tc	961.47	K	Joback Method
tf	438.77	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.91	J/molxK	719.64	Joback Method
cpg	504.02	J/molxK	759.95	Joback Method
cpg	516.98	J/molxK	800.25	Joback Method
cpg	528.84	J/molxK	840.56	Joback Method
cpg	539.64	J/molxK	880.86	Joback Method
cpg	549.44	J/molxK	921.17	Joback Method
cpg	558.27	J/molxK	961.47	Joback Method
dvisc	0.0009123	Paxs	438.77	Joback Method
dvisc	0.0005593	Paxs	485.58	Joback Method

dvisc	0.0003737	Paxs	532.39	Joback Method
dvisc	0.0002665	Paxs	579.20	Joback Method
dvisc	0.0001999	Paxs	626.02	Joback Method
dvisc	0.0001561	Paxs	672.83	Joback Method
dvisc	0.0001259	Paxs	719.64	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=U360526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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