4-Ethylbenzoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C15H13ClO2/c1-2-11-3-5-12(6-4-11)15(17)18-14-9-7-13(16)8-10-14/h3-10H,2
InchiKey: YSLISJQPFLHFPN-UHFFFAOYSA-N
Formula: C15H13ClO2
SMILES: CCc1ccc(C(=O)Oc2ccc(Cl)cc2)cc1
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
mcvol	194.370	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	719.64	K	Joback Method
tc	961.47	K	Joback Method
tf	438.77	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.91	J/mol×K	719.64	Joback Method
cpg	504.02	J/mol×K	759.95	Joback Method
cpg	516.98	J/mol×K	800.25	Joback Method
cpg	528.84	J/mol×K	840.56	Joback Method
cpg	539.64	J/mol×K	880.86	Joback Method
cpg	549.44	J/mol×K	921.17	Joback Method
cpg	558.27	J/mol×K	961.47	Joback Method
dvisc	0.0009123	Pa×s	438.77	Joback Method

dvisc	0.0005593	Pa×s	485.58	Joback Method
dvisc	0.0003737	Pa×s	532.39	Joback Method
dvisc	0.0002665	Pa×s	579.20	Joback Method
dvisc	0.0001999	Pa×s	626.02	Joback Method
dvisc	0.0001561	Pa×s	672.83	Joback Method
dvisc	0.0001259	Pa×s	719.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307122&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