4-Ethylbenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C15H12Cl2O2/c1-2-10-3-5-11(6-4-10)15(18)19-12-7-8-13(16)14(17)9-12/h3-9H
InchiKey: UHVGMXBIDBHYKS-UHFFFAOYSA-N
Formula: C15H12Cl2O2
SMILES: CCc1ccc(C(=O)Oc2ccc(Cl)c(Cl)c2)cc1
Mol. weight [g/mol]: 295.16

Physical Properties

Property code	Value	Unit	Source
gf	13.57	kJ/mol	Joback Method
hf	-190.56	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.775		Crippen Method
mcvol	206.610	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	2251.00		NIST Webbook
tb	762.05	K	Joback Method
tc	1006.83	K	Joback Method
tf	481.21	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.80	J/mol×K	762.05	Joback Method
cpg	524.49	J/mol×K	802.85	Joback Method
cpg	536.08	J/mol×K	843.64	Joback Method
cpg	546.62	J/mol×K	884.44	Joback Method
cpg	556.14	J/mol×K	925.24	Joback Method
cpg	564.68	J/mol×K	966.03	Joback Method
cpg	572.29	J/mol×K	1006.83	Joback Method
dvisc	0.0006936	Pa×s	481.21	Joback Method
dvisc	0.0004502	Pa×s	528.02	Joback Method

dvisc	0.0003135	Pa×s	574.82	Joback Method
dvisc	0.0002305	Pa×s	621.63	Joback Method
dvisc	0.0001770	Pa×s	668.44	Joback Method
dvisc	0.0001406	Pa×s	715.24	Joback Method
dvisc	0.0001150	Pa×s	762.05	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=U307126&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

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