2-Fluorobenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H7Cl2FO2/c14-10-6-5-8(7-11(10)15)18-13(17)9-3-1-2-4-12(9)16/h1-7H
InchiKey: ODWCIDDVKYMMDX-UHFFFAOYSA-N
Formula: C13H7Cl2FO2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1ccccc1F
Mol. weight [g/mol]: 285.10

Physical Properties

Property code	Value	Unit	Source
gf	-198.08	kJ/mol	Joback Method
hf	-345.39	kJ/mol	Joback Method
hfus	30.60	kJ/mol	Joback Method
hvap	68.18	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.352		Crippen Method
mcvol	180.200	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	715.56	K	Joback Method
tc	959.61	K	Joback Method
tf	459.26	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.98	J/mol×K	715.56	Joback Method
cpg	428.00	J/mol×K	756.24	Joback Method
cpg	438.06	J/mol×K	796.91	Joback Method
cpg	447.19	J/mol×K	837.59	Joback Method
cpg	455.42	J/mol×K	878.26	Joback Method
cpg	462.77	J/mol×K	918.94	Joback Method
cpg	469.29	J/mol×K	959.61	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=U307690&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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