3,4-Difluorobenzoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C13H7ClF2O2/c14-9-2-4-10(5-3-9)18-13(17)8-1-6-11(15)12(16)7-8/h1-7H
InchiKey: URZRXXYRJUIMNR-UHFFFAOYSA-N
Formula: C13H7ClF2O2
SMILES: O=C(Oc1ccc(Cl)cc1)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 268.64

Physical Properties

Property code	Value	Unit	Source
gf	-380.96	kJ/mol	Joback Method
hf	-525.76	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.837		Crippen Method
mcvol	169.730	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	677.40	K	Joback Method
tc	908.05	K	Joback Method
tf	429.93	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.10	J/mol×K	677.40	Joback Method
cpg	414.64	J/mol×K	715.84	Joback Method
cpg	425.29	J/mol×K	754.28	Joback Method
cpg	435.06	J/mol×K	792.72	Joback Method
cpg	443.98	J/mol×K	831.16	Joback Method
cpg	452.08	J/mol×K	869.61	Joback Method
cpg	459.38	J/mol×K	908.05	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=U357712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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