2,5-Difluorobenzoic acid, phenyl ester

Inchi: InChI=1S/C13H8F2O2/c14-9-6-7-12(15)11(8-9)13(16)17-10-4-2-1-3-5-10/h1-8H
InchiKey: BGYKTOQZECZEJH-UHFFFAOYSA-N
Formula: C13H8F2O2
SMILES: O=C(Oc1ccccc1)c1cc(F)ccc1F
Mol. weight [g/mol]: 234.20

Physical Properties

Property code	Value	Unit	Source
gf	-359.40	kJ/mol	Joback Method
hf	-498.55	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.184		Crippen Method
mcvol	157.490	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1659.00		NIST Webbook
tb	634.99	K	Joback Method
tc	861.72	K	Joback Method
tf	387.49	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.82	J/mol×K	634.99	Joback Method
cpg	393.64	J/mol×K	672.78	Joback Method
cpg	405.52	J/mol×K	710.57	Joback Method
cpg	416.49	J/mol×K	748.35	Joback Method
cpg	426.58	J/mol×K	786.14	Joback Method
cpg	435.82	J/mol×K	823.93	Joback Method
cpg	444.24	J/mol×K	861.72	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=U357576&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