Phenylacetic acid, 3,5-difluorophenyl ester

Inchi: InChI=1S/C14H10F2O2/c15-11-7-12(16)9-13(8-11)18-14(17)6-10-4-2-1-3-5-10/h1-5,7-9H
InchiKey: MPVTYZFAJKBWPY-UHFFFAOYSA-N
Formula: C14H10F2O2
SMILES: O=C(Cc1ccccc1)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 248.22

Physical Properties

Property code	Value	Unit	Source
gf	-350.98	kJ/mol	Joback Method
hf	-519.19	kJ/mol	Joback Method
hfus	28.27	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.113		Crippen Method
mcvol	171.580	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
tb	657.87	K	Joback Method
tc	880.43	K	Joback Method
tf	398.76	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.13	J/mol×K	657.87	Joback Method
cpg	443.56	J/mol×K	694.96	Joback Method
cpg	456.02	J/mol×K	732.06	Joback Method
cpg	467.55	J/mol×K	769.15	Joback Method
cpg	478.16	J/mol×K	806.24	Joback Method
cpg	487.90	J/mol×K	843.34	Joback Method
cpg	496.80	J/mol×K	880.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299002&Units=SI
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

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