3-Phenylpropionic acid. 3,5-difluorophenyl ester

Inchi: InChI=1S/C15H12F2O2/c16-12-8-13(17)10-14(9-12)19-15(18)7-6-11-4-2-1-3-5-11/h1-5,8

InchiKey: ULUXOHUBNMTRAG-UHFFFAOYSA-N

Formula: C15H12F2O2

SMILES: O=C(CCc1ccccc1)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 262.25

Physical Properties

Property code	Value	Unit	Source
gf	-342.56	kJ/mol	Joback Method
hf	-539.83	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	62.38	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.503		Crippen Method
mcvol	185.670	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	680.75	K	Joback Method
tc	899.48	K	Joback Method
tf	410.03	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.84	J/mol×K	680.75	Joback Method
cpg	494.78	J/mol×K	717.20	Joback Method
cpg	507.73	J/mol×K	753.66	Joback Method
cpg	519.72	J/mol×K	790.11	Joback Method
cpg	530.77	J/mol×K	826.57	Joback Method
cpg	540.94	J/mol×K	863.02	Joback Method
cpg	550.24	J/mol×K	899.48	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=U299020&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