Butyric acid, 2-phenyl-, 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H15F3O2/c1-3-11(10-7-5-4-6-8-10)12(17)18-9(2)13(14,15)16/h4-9,11H,3H

InchiKey: YDRHIWSKEIHPHF-UHFFFAOYSA-N

Formula: C13H15F3O2

SMILES: CCC(C(=O)OC(C)C(F)(F)F)c1ccccc1

Mol. weight [g/mol]: 260.25

Physical Properties

Property code	Value	Unit	Source
gf	-649.40	kJ/mol	Joback Method
hf	-927.56	kJ/mol	Joback Method
hfus	21.03	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.674		Crippen Method
mcvol	183.020	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
tb	593.51	K	Joback Method
tc	788.14	K	Joback Method
tf	309.04	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.63	J/mol×K	593.51	Joback Method
cpg	486.76	J/mol×K	625.95	Joback Method
cpg	500.94	J/mol×K	658.39	Joback Method
cpg	514.21	J/mol×K	690.83	Joback Method
cpg	526.61	J/mol×K	723.26	Joback Method
cpg	538.19	J/mol×K	755.70	Joback Method
cpg	548.97	J/mol×K	788.14	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=U406851&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