Butyric acid, 2-phenyl-, 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H14F4O2/c1-2-10(9-6-4-3-5-7-9)11(18)19-8-13(16,17)12(14)15/h3-7,10,12

InchiKey: HDDMAXKBAVFEMN-UHFFFAOYSA-N

Formula: C13H14F4O2

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

Mol. weight [g/mol]: 278.24

Physical Properties

Property code	Value	Unit	Source
gf	-844.21	kJ/mol	Joback Method
hf	-1123.67	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	50.62	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.624		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
tb	592.78	K	Joback Method
tc	779.13	K	Joback Method
tf	309.63	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.76	J/mol×K	592.78	Joback Method
cpg	494.22	J/mol×K	623.84	Joback Method
cpg	507.80	J/mol×K	654.90	Joback Method
cpg	520.53	J/mol×K	685.95	Joback Method
cpg	532.46	J/mol×K	717.01	Joback Method
cpg	543.61	J/mol×K	748.07	Joback Method
cpg	554.01	J/mol×K	779.13	Joback Method

Sources

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=U406852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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