Butyric acid, 2-phenyl-, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C15H14F8O2/c1-2-10(9-6-4-3-5-7-9)11(24)25-8-13(18,19)15(22,23)14(20,21)1

InchiKey: ZPVMNKRYAMXSJY-UHFFFAOYSA-N

Formula: C15H14F8O2

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

Mol. weight [g/mol]: 378.26

Physical Properties

Property code	Value	Unit	Source
gf	-1600.93	kJ/mol	Joback Method
hf	-1966.89	kJ/mol	Joback Method
hfus	26.79	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.894		Crippen Method
mcvol	220.050	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook
tb	629.16	K	Joback Method
tc	801.64	K	Joback Method
tf	339.37	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.01	J/mol×K	629.16	Joback Method
cpg	634.15	J/mol×K	657.91	Joback Method
cpg	647.33	J/mol×K	686.65	Joback Method
cpg	659.60	J/mol×K	715.40	Joback Method
cpg	671.03	J/mol×K	744.15	Joback Method
cpg	681.66	J/mol×K	772.90	Joback Method
cpg	691.56	J/mol×K	801.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406853&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

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