3-Phenylpropionic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C14H12F8O2/c15-11(16)13(19,20)14(21,22)12(17,18)8-24-10(23)7-6-9-4-2-1-3

InchiKey: PZWWDCHGPGLXKZ-UHFFFAOYSA-N

Formula: C14H12F8O2

SMILES: O=C(CCc1ccccc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 364.23

Physical Properties

Property code	Value	Unit	Source
gf	-1606.91	kJ/mol	Joback Method
hf	-1940.97	kJ/mol	Joback Method
hfus	27.72	kJ/mol	Joback Method
hvap	47.38	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.333		Crippen Method
mcvol	205.960	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
tb	606.72	K	Joback Method
tc	777.29	K	Joback Method
tf	343.10	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.30	J/mol×K	606.72	Joback Method
cpg	581.85	J/mol×K	635.15	Joback Method
cpg	594.48	J/mol×K	663.58	Joback Method
cpg	606.24	J/mol×K	692.01	Joback Method
cpg	617.18	J/mol×K	720.44	Joback Method
cpg	627.36	J/mol×K	748.86	Joback Method
cpg	636.82	J/mol×K	777.29	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=U354734&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