1-Phenylethanol, heptafluorobutyrate

Inchi: InChI=1S/C12H9F7O2/c1-7(8-5-3-2-4-6-8)21-9(20)10(13,14)11(15,16)12(17,18)19/h2-7H
InchiKey: KJGMUECEJSEERZ-UHFFFAOYSA-N
Formula: C12H9F7O2
SMILES: CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 318.19
CAS: 942606-93-1

Physical Properties

Property code	Value	Unit	Source
gf	-1428.94	kJ/mol	Joback Method
hf	-1703.58	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	43.74	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.124		Crippen Method
mcvol	176.010	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
tb	561.69	K	Joback Method
tc	741.78	K	Joback Method
tf	319.97	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.49	J/mol×K	561.69	Joback Method
cpg	474.82	J/mol×K	591.70	Joback Method
cpg	487.17	J/mol×K	621.72	Joback Method
cpg	498.59	J/mol×K	651.73	Joback Method
cpg	509.13	J/mol×K	681.75	Joback Method
cpg	518.86	J/mol×K	711.76	Joback Method
cpg	527.83	J/mol×K	741.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C942606931&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