Pentadecafluorooctanoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C21H11F15O3/c22-15(23,14(37)39-13-8-6-12(7-9-13)38-10-11-4-2-1-3-5-11)1

InchiKey: KUVCRZQYGASDAZ-UHFFFAOYSA-N

Formula: C21H11F15O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 596.29

Physical Properties

Property code	Value	Unit	Source
gf	-2900.06	kJ/mol	Joback Method
hf	-3395.10	kJ/mol	Joback Method
hfus	36.12	kJ/mol	Joback Method
hvap	57.79	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	7.545		Crippen Method
mcvol	299.090	ml/mol	McGowan Method
pc	1040.58	kPa	Joback Method
rinpol	1863.00		NIST Webbook
tb	803.37	K	Joback Method
tc	988.19	K	Joback Method
tf	511.97	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.27	J/mol×K	803.37	Joback Method
cpg	958.29	J/mol×K	834.17	Joback Method
cpg	968.39	J/mol×K	864.98	Joback Method
cpg	977.70	J/mol×K	895.78	Joback Method
cpg	986.34	J/mol×K	926.58	Joback Method
cpg	994.44	J/mol×K	957.38	Joback Method
cpg	1002.13	J/mol×K	988.19	Joback Method

Sources

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=U406894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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