2-(2-Ethoxyethoxy)ethyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C13H13F5O4/c1-2-20-3-4-21-5-6-22-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h

InchiKey: SZCGRTKSXWGXPC-UHFFFAOYSA-N

Formula: C13H13F5O4

SMILES: CCOCCOCCOC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 328.23

Physical Properties

Property code	Value	Unit	Source
gf	-1295.13	kJ/mol	Joback Method
hf	-1622.26	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.592		Crippen Method
mcvol	198.300	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	665.90	K	Joback Method
tc	836.54	K	Joback Method
tf	444.86	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.20	J/mol×K	665.90	Joback Method
cpg	544.99	J/mol×K	694.34	Joback Method
cpg	556.26	J/mol×K	722.78	Joback Method
cpg	567.00	J/mol×K	751.22	Joback Method
cpg	577.19	J/mol×K	779.66	Joback Method
cpg	586.83	J/mol×K	808.10	Joback Method
cpg	595.89	J/mol×K	836.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378302&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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