2-Ethoxyethyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C11H9F5O3/c1-2-18-3-4-19-11(17)5-6(12)8(14)10(16)9(15)7(5)13/h2-4H2,1H3
InchiKey: UNGUNUQFXUDKAP-UHFFFAOYSA-N
Formula: C11H9F5O3
SMILES: CCOCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 284.18

Physical Properties

Property code	Value	Unit	Source
gf	-1206.97	kJ/mol	Joback Method
hf	-1448.76	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	53.15	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.575		Crippen Method
mcvol	164.250	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
tb	597.72	K	Joback Method
tc	768.98	K	Joback Method
tf	400.09	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.28	J/mol×K	597.72	Joback Method
cpg	419.59	J/mol×K	626.26	Joback Method
cpg	429.51	J/mol×K	654.81	Joback Method
cpg	439.03	J/mol×K	683.35	Joback Method
cpg	448.13	J/mol×K	711.90	Joback Method
cpg	456.80	J/mol×K	740.44	Joback Method
cpg	465.04	J/mol×K	768.98	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=U378297&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