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

Inchi: InChI=1S/C13H13F5O3/c1-2-3-4-20-5-6-21-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h2-6
InchiKey: DISSZLWHURWYTK-UHFFFAOYSA-N
Formula: C13H13F5O3
SMILES: CCCCOCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 312.23

Physical Properties

Property code	Value	Unit	Source
gf	-1190.13	kJ/mol	Joback Method
hf	-1490.04	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	57.60	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.356		Crippen Method
mcvol	192.430	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1507.00		NIST Webbook
tb	643.48	K	Joback Method
tc	813.62	K	Joback Method
tf	422.63	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.36	J/mol×K	643.48	Joback Method
cpg	519.18	J/mol×K	671.84	Joback Method
cpg	530.50	J/mol×K	700.19	Joback Method
cpg	541.30	J/mol×K	728.55	Joback Method
cpg	551.59	J/mol×K	756.91	Joback Method
cpg	561.35	J/mol×K	785.26	Joback Method
cpg	570.59	J/mol×K	813.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378295&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