2-(2-(2-Butoxyethoxy)ethoxy)ethyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C17H21F5O5/c1-2-3-4-24-5-6-25-7-8-26-9-10-27-17(23)11-12(18)14(20)16(22

InchiKey: CGCMKWRUMYSZEB-UHFFFAOYSA-N

Formula: C17H21F5O5

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

Mol. weight [g/mol]: 400.34

Physical Properties

Property code	Value	Unit	Source
gf	-1366.45	kJ/mol	Joback Method
hf	-1837.04	kJ/mol	Joback Method
hfus	53.63	kJ/mol	Joback Method
hvap	71.32	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.389		Crippen Method
mcvol	260.530	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	2033.00		NIST Webbook
tb	779.84	K	Joback Method
tc	957.89	K	Joback Method
tf	512.17	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.93	J/mol×K	779.84	Joback Method
cpg	791.93	J/mol×K	809.51	Joback Method
cpg	805.10	J/mol×K	839.19	Joback Method
cpg	817.40	J/mol×K	868.86	Joback Method
cpg	828.82	J/mol×K	898.54	Joback Method
cpg	839.35	J/mol×K	928.21	Joback Method
cpg	848.97	J/mol×K	957.89	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=U378304&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