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

Inchi: InChI=1S/C15H17F5O4/c1-2-3-4-22-5-6-23-7-8-24-15(21)9-10(16)12(18)14(20)13(19)11

InchiKey: VDNGUFAWXMSFGQ-UHFFFAOYSA-N

Formula: C15H17F5O4

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

Mol. weight [g/mol]: 356.29

Physical Properties

Property code	Value	Unit	Source
gf	-1278.29	kJ/mol	Joback Method
hf	-1663.54	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	64.46	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.372		Crippen Method
mcvol	226.480	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	1770.00		NIST Webbook
tb	711.66	K	Joback Method
tc	883.52	K	Joback Method
tf	467.40	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.79	J/mol×K	711.66	Joback Method
cpg	651.81	J/mol×K	740.30	Joback Method
cpg	664.19	J/mol×K	768.95	Joback Method
cpg	675.92	J/mol×K	797.59	Joback Method
cpg	686.99	J/mol×K	826.23	Joback Method
cpg	697.39	J/mol×K	854.87	Joback Method
cpg	707.10	J/mol×K	883.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378300&Units=SI

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

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