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

Inchi: InChI=1S/C14H15F5O5/c1-21-2-3-22-4-5-23-6-7-24-14(20)8-9(15)11(17)13(19)12(18)10

InchiKey: HENMLTRBSZOUSW-UHFFFAOYSA-N

Formula: C14H15F5O5

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

Mol. weight [g/mol]: 358.26

Physical Properties

Property code	Value	Unit	Source
gf	-1391.71	kJ/mol	Joback Method
hf	-1775.12	kJ/mol	Joback Method
hfus	45.86	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.218		Crippen Method
mcvol	218.260	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	711.20	K	Joback Method
tc	883.44	K	Joback Method
tf	478.36	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.14	J/mol×K	711.20	Joback Method
cpg	624.52	J/mol×K	739.91	Joback Method
cpg	636.29	J/mol×K	768.61	Joback Method
cpg	647.43	J/mol×K	797.32	Joback Method
cpg	657.91	J/mol×K	826.03	Joback Method
cpg	667.71	J/mol×K	854.73	Joback Method
cpg	676.82	J/mol×K	883.44	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=U378303&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