2,5,8,11-Tetraoxatridecan-13-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C16H19F5O6/c1-23-2-3-24-4-5-25-6-7-26-8-9-27-16(22)10-11(17)13(19)15(21

InchiKey: SIBNAOBOEUIEEN-UHFFFAOYSA-N

Formula: C16H19F5O6

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

Mol. weight [g/mol]: 402.31

Physical Properties

Property code	Value	Unit	Source
gf	-1479.87	kJ/mol	Joback Method
hf	-1948.62	kJ/mol	Joback Method
hfus	52.23	kJ/mol	Joback Method
hvap	71.51	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.235		Crippen Method
mcvol	252.310	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2064.00		NIST Webbook
tb	779.38	K	Joback Method
tc	957.59	K	Joback Method
tf	523.13	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.71	J/mol×K	779.38	Joback Method
cpg	763.09	J/mol×K	809.08	Joback Method
cpg	775.64	J/mol×K	838.78	Joback Method
cpg	787.32	J/mol×K	868.48	Joback Method
cpg	798.11	J/mol×K	898.18	Joback Method
cpg	807.97	J/mol×K	927.88	Joback Method
cpg	816.89	J/mol×K	957.59	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=U378299&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