2-(2-Isopentoxyethoxy)ethyl trifluoroacetate

Inchi: InChI=1S/C11H19F3O4/c1-9(2)3-4-16-5-6-17-7-8-18-10(15)11(12,13)14/h9H,3-8H2,1-2H
InchiKey: CVZPXTWVZFDHBO-UHFFFAOYSA-N
Formula: C11H19F3O4
SMILES: CC(C)CCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 272.26

Physical Properties

Property code	Value	Unit	Source
gf	-986.21	kJ/mol	Joback Method
hf	-1381.97	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	49.92	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	2.171		Crippen Method
mcvol	190.340	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1296.40		NIST Webbook
rinpol	1296.40		NIST Webbook
tb	566.35	K	Joback Method
tc	727.63	K	Joback Method
tf	319.54	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.13	J/mol×K	566.35	Joback Method
cpg	510.96	J/mol×K	593.23	Joback Method
cpg	524.24	J/mol×K	620.11	Joback Method
cpg	536.96	J/mol×K	646.99	Joback Method
cpg	549.13	J/mol×K	673.87	Joback Method
cpg	560.76	J/mol×K	700.75	Joback Method
cpg	571.85	J/mol×K	727.63	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=R188760&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