2-(2-Pentoxyethoxy)ethyl trifluoroacetate

Inchi: InChI=1S/C11H19F3O4/c1-2-3-4-5-16-6-7-17-8-9-18-10(15)11(12,13)14/h2-9H2,1H3
InchiKey: YCERBFPMLMMKKS-UHFFFAOYSA-N
Formula: C11H19F3O4
SMILES: CCCCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 272.26

Physical Properties

Property code	Value	Unit	Source
gf	-983.77	kJ/mol	Joback Method
hf	-1376.69	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	50.31	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.315		Crippen Method
mcvol	190.340	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
tb	566.79	K	Joback Method
tc	725.57	K	Joback Method
tf	334.54	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.80	J/mol×K	566.79	Joback Method
cpg	510.37	J/mol×K	593.25	Joback Method
cpg	523.41	J/mol×K	619.72	Joback Method
cpg	535.91	J/mol×K	646.18	Joback Method
cpg	547.89	J/mol×K	672.65	Joback Method
cpg	559.35	J/mol×K	699.11	Joback Method
cpg	570.28	J/mol×K	725.57	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=R188804&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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