2-[2-(2-Pentoxyethoxy)ethoxy]ethyl trifluoroacetate

Inchi: InChI=1S/C13H23F3O5/c1-2-3-4-5-18-6-7-19-8-9-20-10-11-21-12(17)13(14,15)16/h2-11

InchiKey: HSSPOOSWARRFIM-UHFFFAOYSA-N

Formula: C13H23F3O5

SMILES: CCCCCOCCOCCOCCOC(=O)C(F)(F)F

Mol. weight [g/mol]: 316.31

Physical Properties

Property code	Value	Unit	Source
gf	-1071.93	kJ/mol	Joback Method
hf	-1550.19	kJ/mol	Joback Method
hfus	37.60	kJ/mol	Joback Method
hvap	57.17	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	2.332		Crippen Method
mcvol	224.390	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	1575.30		NIST Webbook
tb	634.97	K	Joback Method
tc	794.91	K	Joback Method
tf	379.31	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.83	J/mol×K	634.97	Joback Method
cpg	642.53	J/mol×K	661.63	Joback Method
cpg	656.61	J/mol×K	688.28	Joback Method
cpg	670.08	J/mol×K	714.94	Joback Method
cpg	682.93	J/mol×K	741.60	Joback Method
cpg	695.17	J/mol×K	768.25	Joback Method
cpg	706.80	J/mol×K	794.91	Joback Method

Sources

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=R188671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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