2-[2-(2-Methoxyethoxy)ethoxy]ethyl 2,2,2-trifluoroacetate

Other names: Triethylene glycol monomethyl ether, trifluoroacetate
3,6,9-Trioxadeca-1-yl trifluoroacetate

Inchi: InChI=1S/C9H15F3O5/c1-14-2-3-15-4-5-16-6-7-17-8(13)9(10,11)12/h2-7H2,1H3

InchiKey: CHICNFUCCDFSPQ-UHFFFAOYSA-N

Formula: C9H15F3O5

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

Mol. weight [g/mol]: 260.21

Physical Properties

Property code	Value	Unit	Source
gf	-1105.61	kJ/mol	Joback Method
hf	-1467.63	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	48.27	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	0.772		Crippen Method
mcvol	168.030	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1228.60		NIST Webbook
rinpol	1228.60		NIST Webbook
tb	543.45	K	Joback Method
tc	703.23	K	Joback Method
tf	334.23	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.41	J/mol×K	543.45	Joback Method
cpg	438.36	J/mol×K	570.08	Joback Method
cpg	449.90	J/mol×K	596.71	Joback Method
cpg	461.01	J/mol×K	623.34	Joback Method
cpg	471.68	J/mol×K	649.97	Joback Method
cpg	481.92	J/mol×K	676.60	Joback Method

cpg	491.71	J/mol×K	703.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351955&Units=SI
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

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

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