

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

Other names:	Tetraethylene glycol monomethyl ether, trifluoroacetate 3,6,9,12-Tetraoxatridec-1-yl trifluoroacetate
Inchi:	InChI=1S/C11H19F3O6/c1-16-2-3-17-4-5-18-6-7-19-8-9-20-10(15)11(12,13)14/h2-9H2,1
InchiKey:	RIGBFMIXMQBWBE-UHFFFAOYSA-N
Formula:	C11H19F3O6
SMILES:	COCCOCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	304.26

Physical Properties

Property code	Value	Unit	Source
gf	-1193.77	kJ/mol	Joback Method
hf	-1641.13	kJ/mol	Joback Method
hfus	33.61	kJ/mol	Joback Method
hvap	55.13	kJ/mol	Joback Method
log10ws	-0.30		Crippen Method
logp	0.788		Crippen Method
mcvol	202.080	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1473.60		NIST Webbook
rinpol	1473.60		NIST Webbook
tb	611.63	K	Joback Method
tc	771.56	K	Joback Method
tf	379.00	K	Joback Method
vc	0.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.14	J/molxK	611.63	Joback Method
cpg	564.50	J/molxK	638.28	Joback Method
cpg	577.34	J/molxK	664.94	Joback Method
cpg	589.66	J/molxK	691.59	Joback Method
cpg	601.44	J/molxK	718.25	Joback Method
cpg	612.67	J/molxK	744.90	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=U351956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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