

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

Other names: Triethylene glycol monoethyl ether, trifluoroacetate
3,6,9-Trioxaundec-1-yl trifluoroacetate

Inchi: InChI=1S/C10H17F3O5/c1-2-15-3-4-16-5-6-17-7-8-18-9(14)10(11,12)13/h2-8H2,1H3

InchiKey: BEWZRKTZWUVJLZ-UHFFFAOYSA-N

Formula: C10H17F3O5

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

Mol. weight [g/mol]: 274.23

Physical Properties

Property code	Value	Unit	Source
gf	-1097.19	kJ/mol	Joback Method
hf	-1488.27	kJ/mol	Joback Method
hfus	29.83	kJ/mol	Joback Method
hvap	50.49	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	1.162		Crippen Method
mcvol	182.120	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1278.00		NIST Webbook
tb	566.33	K	Joback Method
tc	725.73	K	Joback Method
tf	345.50	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.31	J/mol×K	566.33	Joback Method
cpg	487.05	J/mol×K	592.90	Joback Method
cpg	499.31	J/mol×K	619.46	Joback Method
cpg	511.10	J/mol×K	646.03	Joback Method
cpg	522.40	J/mol×K	672.59	Joback Method
cpg	533.22	J/mol×K	699.16	Joback Method
cpg	543.56	J/mol×K	725.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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