2-[2-(2,2,2-Trifluoroacetyl)oxyethoxy]ethyl 2,2,2-trifluoroacetate

Other names: Diethylene glycol, bis(trifluoroacetate)
8,8,8-Trifluoro-7-oxo-3,6-dioxaoct-1-yl trifluoroacetate

Inchi: InChI=1S/C8H8F6O5/c9-7(10,11)5(15)18-3-1-17-2-4-19-6(16)8(12,13)14/h1-4H2

InchiKey: DTPMBHDSZMCYBV-UHFFFAOYSA-N

Formula: C8H8F6O5

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

Mol. weight [g/mol]: 298.14

Physical Properties

Property code	Value	Unit	Source
gf	-1719.54	kJ/mol	Joback Method
hf	-2024.43	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	46.63	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.214		Crippen Method
mcvol	154.950	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1037.60		NIST Webbook
tb	546.60	K	Joback Method
tc	703.83	K	Joback Method
tf	354.85	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.49	J/mol×K	546.60	Joback Method
cpg	412.29	J/mol×K	572.81	Joback Method
cpg	421.62	J/mol×K	599.01	Joback Method
cpg	430.48	J/mol×K	625.22	Joback Method
cpg	438.87	J/mol×K	651.42	Joback Method
cpg	446.82	J/mol×K	677.63	Joback Method
cpg	454.32	J/mol×K	703.83	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=U351951&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

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