2-(2,2,2-Trifluoroacetyl)oxyethyl 2,2,2-trifluoroacetate

Other names: Ethylene glycol, bis(trifluoroacetate)
Acetic acid, trifluoro-, ethylene ester

Inchi: InChI=1S/C6H4F6O4/c7-5(8,9)3(13)15-1-2-16-4(14)6(10,11)12/h1-2H2

InchiKey: CXCMIWOFWYPWSS-UHFFFAOYSA-N

Formula: C6H4F6O4

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

Mol. weight [g/mol]: 254.08

Physical Properties

Property code	Value	Unit	Source
gf	-1631.38	kJ/mol	Joback Method
hf	-1850.93	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	39.77	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.197		Crippen Method
mcvol	120.900	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	780.30		NIST Webbook
tb	478.42	K	Joback Method
tc	636.43	K	Joback Method
tf	310.08	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.23	J/mol×K	478.42	Joback Method
cpg	301.56	J/mol×K	504.75	Joback Method
cpg	309.46	J/mol×K	531.09	Joback Method
cpg	316.92	J/mol×K	557.42	Joback Method
cpg	323.96	J/mol×K	583.76	Joback Method
cpg	330.60	J/mol×K	610.09	Joback Method
cpg	336.84	J/mol×K	636.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351900&Units=SI

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