2-(2-Hydroxyethoxy)ethyl 2,2,2-trifluoroacetate

Other names: Diethylene glycol, mono(trifluoroacetate)
Inchi: InChI=1S/C6H9F3O4/c7-6(8,9)5(11)13-4-3-12-2-1-10/h10H,1-4H2
InchiKey: XHCFUEDTUDBMFR-UHFFFAOYSA-N
Formula: C6H9F3O4
SMILES: O=C(OCCOCCO)C(F)(F)F
Mol. weight [g/mol]: 202.13

Physical Properties

Property code	Value	Unit	Source
gf	-1057.69	kJ/mol	Joback Method
hf	-1293.50	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.101		Crippen Method
mcvol	119.890	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	997.90		NIST Webbook
rinpol	997.90		NIST Webbook
tb	522.15	K	Joback Method
tc	679.99	K	Joback Method
tf	316.78	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.08	J/mol×K	522.15	Joback Method
cpg	304.33	J/mol×K	548.46	Joback Method
cpg	312.24	J/mol×K	574.76	Joback Method
cpg	319.81	J/mol×K	601.07	Joback Method
cpg	327.05	J/mol×K	627.38	Joback Method
cpg	333.95	J/mol×K	653.68	Joback Method
cpg	340.54	J/mol×K	679.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351923&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

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