2,2',2''-Nitrilotriethanol, O, O'-bis(trifluoroacetyl)

Other names: [(2-Hydroxyethyl)azanediyl]bis(ethane-2,1-diyl) bis(2,2,2-trifluoroacetate)
Inchi: InChI=1S/C10H13F6NO5/c11-9(12,13)7(19)21-5-2-17(1-4-18)3-6-22-8(20)10(14,15)16/h
InchiKey: JOGYYXONGISBQT-UHFFFAOYSA-N
Formula: C10H13F6NO5
SMILES: O=C(OCCN(CCO)CCOC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 341.20

Physical Properties

Property code	Value	Unit	Source
gf	-1623.74	kJ/mol	Joback Method
hf	-2018.19	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.492		Crippen Method
mcvol	193.110	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
tb	674.56	K	Joback Method
tc	833.85	K	Joback Method
tf	448.45	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.04	J/mol×K	674.56	Joback Method
cpg	574.09	J/mol×K	701.11	Joback Method
cpg	583.56	J/mol×K	727.66	Joback Method
cpg	592.47	J/mol×K	754.20	Joback Method
cpg	600.84	J/mol×K	780.75	Joback Method
cpg	608.69	J/mol×K	807.30	Joback Method
cpg	616.05	J/mol×K	833.85	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=U378720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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