Ethanolamine, N,O-bis(trifluoroacetyl)-

Inchi: InChI=1S/C6H5F6NO3/c7-5(8,9)3(14)13-1-2-16-4(15)6(10,11)12/h1-2H2,(H,13,14)
InchiKey: YDQHOULJYAFDRM-UHFFFAOYSA-N
Formula: C6H5F6NO3
SMILES: O=C(NCCOC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 253.10

Physical Properties

Property code	Value	Unit	Source
gf	-1436.99	kJ/mol	Joback Method
hf	-1665.24	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	43.79	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	0.770		Crippen Method
mcvol	125.010	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	945.00		NIST Webbook
tb	506.17	K	Joback Method
tc	667.73	K	Joback Method
tf	340.51	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.43	J/mol×K	506.17	Joback Method
cpg	322.18	J/mol×K	533.10	Joback Method
cpg	330.40	J/mol×K	560.02	Joback Method
cpg	338.12	J/mol×K	586.95	Joback Method
cpg	345.35	J/mol×K	613.88	Joback Method
cpg	352.11	J/mol×K	640.80	Joback Method
cpg	358.42	J/mol×K	667.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375585&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume