1,1-Diethoxy-2,2,2-trifluoro-1-(ethylthio)ethane

Inchi: InChI=1S/C8H15F3O2S/c1-4-12-8(13-5-2,14-6-3)7(9,10)11/h4-6H2,1-3H3
InchiKey: UURXWCXKJIPEMW-UHFFFAOYSA-N
Formula: C8H15F3O2S
SMILES: CCOC(OCC)(SCC)C(F)(F)F
Mol. weight [g/mol]: 232.26
CAS: 68058-56-0

Physical Properties

Property code	Value	Unit	Source
gf	-739.15	kJ/mol	Joback Method
hf	-1066.00 ± 11.00	kJ/mol	NIST Webbook
hfus	17.39	kJ/mol	Joback Method
hvap	40.00	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.029		Crippen Method
mcvol	156.980	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	487.41	K	Joback Method
tc	665.91	K	Joback Method
tf	265.39	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.07	J/mol×K	487.41	Joback Method
cpg	380.63	J/mol×K	517.16	Joback Method
cpg	393.52	J/mol×K	546.91	Joback Method
cpg	405.77	J/mol×K	576.66	Joback Method
cpg	417.38	J/mol×K	606.41	Joback Method
cpg	428.38	J/mol×K	636.16	Joback Method
cpg	438.78	J/mol×K	665.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68058560&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume