2-(2-Isobutoxyethoxy)ethyl trifluroacetate

Inchi: InChI=1S/C10H17F3O4/c1-8(2)7-16-4-3-15-5-6-17-9(14)10(11,12)13/h8H,3-7H2,1-2H3
InchiKey: DEQJNTWHUPACAN-UHFFFAOYSA-N
Formula: C10H17F3O4
SMILES: CC(C)COCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 258.23

Physical Properties

Property code	Value	Unit	Source
gf	-994.63	kJ/mol	Joback Method
hf	-1361.33	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.781		Crippen Method
mcvol	176.250	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
tb	543.47	K	Joback Method
tc	705.27	K	Joback Method
tf	308.27	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.35	J/mol×K	543.47	Joback Method
cpg	461.48	J/mol×K	570.44	Joback Method
cpg	474.09	J/mol×K	597.40	Joback Method
cpg	486.20	J/mol×K	624.37	Joback Method
cpg	497.79	J/mol×K	651.34	Joback Method
cpg	508.88	J/mol×K	678.31	Joback Method
cpg	519.46	J/mol×K	705.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188720&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