2-(2-Butoxyethoxy)ethyl 2,2,2-trifluoroacetate

Other names: Diethylene glycol butyl ether, trifluoroacetate
3,6-Dioxaodec-1-yl trifluoroacetate
Inchi: InChI=1S/C10H17F3O4/c1-2-3-4-15-5-6-16-7-8-17-9(14)10(11,12)13/h2-8H2,1H3
InchiKey: PITLYPONAMTONM-UHFFFAOYSA-N
Formula: C10H17F3O4
SMILES: CCCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 258.23

Physical Properties

Property code	Value	Unit	Source
gf	-992.19	kJ/mol	Joback Method
hf	-1356.05	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	48.08	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.925		Crippen Method
mcvol	176.250	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1199.60		NIST Webbook
rinpol	1221.80		NIST Webbook
rinpol	1199.60		NIST Webbook
rinpol	1221.80		NIST Webbook
tb	543.91	K	Joback Method
tc	703.03	K	Joback Method
tf	323.27	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.05	J/mol×K	543.91	Joback Method
cpg	460.91	J/mol×K	570.43	Joback Method
cpg	473.28	J/mol×K	596.95	Joback Method
cpg	485.16	J/mol×K	623.47	Joback Method

cpg	496.54	J/mol×K	649.99	Joback Method
cpg	507.45	J/mol×K	676.51	Joback Method
cpg	517.87	J/mol×K	703.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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