2-Butoxyethyl 2,2,2-trifluoroacetate

Other names: 2-Butoxyethanol, trifluoroacetate
Inchi: InChI=1S/C8H13F3O3/c1-2-3-4-13-5-6-14-7(12)8(9,10)11/h2-6H2,1H3
InchiKey: NIMPJBNMRJJAEE-UHFFFAOYSA-N
Formula: C8H13F3O3
SMILES: CCCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 214.18

Physical Properties

Property code	Value	Unit	Source
gf	-904.03	kJ/mol	Joback Method
hf	-1182.55	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	41.22	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.909		Crippen Method
mcvol	142.200	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	953.70		NIST Webbook
rinpol	948.50		NIST Webbook
rinpol	948.50		NIST Webbook
tb	475.73	K	Joback Method
tc	636.00	K	Joback Method
tf	278.50	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.55	J/mol×K	475.73	Joback Method
cpg	342.94	J/mol×K	502.44	Joback Method
cpg	353.88	J/mol×K	529.15	Joback Method
cpg	364.39	J/mol×K	555.86	Joback Method
cpg	374.47	J/mol×K	582.58	Joback Method
cpg	384.12	J/mol×K	609.29	Joback Method

cpg	393.36	J/mol×K	636.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351933&Units=SI

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