Trifluoroacetic acid, butyl ester

Other names:	Trifluoroacetic acid, n-butyl ester
	Butyl 2,2,2-trifluoroacetate
	1-Butanol, trifluoroacetate
	n-Butyl trifluoroacetate
	Acetic acid, trifluoro-, butyl ester
	CF3CO2(n-C4H9)
	Trifluoroacetic acid, butyl ester
	CF3C(O)O(CH2)3CH3
Inchi:	InChI=1S/C6H9F3O2/c1-2-3-4-11-5(10)6(7,8)9/h2-4H2,1H3
InchiKey:	CLDYDTBRUJPBGU-UHFFFAOYSA-N
Formula:	C6H9F3O2
SMILES:	CCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	170.13

Physical Properties

Property code	Value	Unit	Source
af	0.4060		Cheméo Relay (1.0)
affp	764.80	kJ/mol	NIST Webbook
basg	733.80	kJ/mol	NIST Webbook
hf	-1056.57	kJ/mol	Cheméo Relay (1.0)
hfus	15.91	kJ/mol	Joback Method
hvap	38.29	kJ/mol	Cheméo Relay (1.0)
ie	11.11	eV	Cheméo Relay (1.0)
log10ws	-1.25		Cheméo Relay (1.0)
logp	1.892		Crippen Method
mcvol	108.150	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	678.80		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	654.20		NIST Webbook
rinpol	664.30		NIST Webbook
ripol	814.00		NIST Webbook
ripol	814.00		NIST Webbook
tb	373.30	K	NIST Webbook
tc	495.58	K	Cheméo Relay (1.0)

tf	192.05	K	Cheméo Relay (1.0)
vc	0.405	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.81	J/mol×K	407.55	Joback Method
cpg	236.43	J/mol×K	434.44	Joback Method
cpg	245.63	J/mol×K	461.33	Joback Method
cpg	254.43	J/mol×K	488.23	Joback Method
cpg	262.84	J/mol×K	515.12	Joback Method
cpg	270.88	J/mol×K	542.01	Joback Method
cpg	278.54	J/mol×K	568.90	Joback Method
hvapt	37.80	kJ/mol	360.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C367646&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature

ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume