1-Octyl trifluoroacetate

Other names:	Octyl trifluoroacetate
	Octyl 2,2,2-trifluoroacetate
	1-Octanol, trifluoroacetate
	Acetic acid, trifluoro-, octyl ester
	Trifluoroacetic acid, octyl ester
Inchi:	InChI=1S/C10H17F3O2/c1-2-3-4-5-6-7-8-15-9(14)10(11,12)13/h2-8H2,1H3
InchiKey:	MGRWEFWRZHQSRH-UHFFFAOYSA-N
Formula:	C10H17F3O2
SMILES:	CCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	226.24
CAS:	2561-21-9

Physical Properties

Property code	Value	Unit	Source
gf	-782.19	kJ/mol	Joback Method
hf	-1091.61	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	43.26	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.452		Crippen Method
mcvol	164.510	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1026.30		NIST Webbook
rinpol	1057.10		NIST Webbook
rinpol	1057.10		NIST Webbook
rinpol	1026.30		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1040.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1185.00		NIST Webbook
tb	458.65 ± 1.50	K	NIST Webbook
tc	657.90	K	Joback Method
tf	278.81	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.60	J/mol×K	499.07	Joback Method
cpg	408.88	J/mol×K	525.54	Joback Method
cpg	421.60	J/mol×K	552.01	Joback Method
cpg	433.77	J/mol×K	578.48	Joback Method
cpg	445.40	J/mol×K	604.96	Joback Method
cpg	456.52	J/mol×K	631.43	Joback Method
cpg	467.13	J/mol×K	657.90	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=C2561219&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume