Trifluoroacetic acid,n-tridecyl ester

Other names:	Tridecyl trifluoroacetate
	Tridecyl 2,2,2-trifluoroacetate
	1-Tridecanol, trifluoroacetate
	Trifluoroacetic acid, tridecyl ester
Inchi:	InChI=1S/C15H27F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-14(19)15(16,17)18/h2-13H2,
InchiKey:	DKWJQENYIDPCEX-UHFFFAOYSA-N
Formula:	C15H27F3O2
SMILES:	CCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	296.37
CAS:	53800-02-5

Physical Properties

Property code	Value	Unit	Source
gf	-740.09	kJ/mol	Joback Method
hf	-1194.81	kJ/mol	Joback Method
hfus	39.22	kJ/mol	Joback Method
hvap	54.39	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.403		Crippen Method
mcvol	234.960	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1527.50		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	613.47	K	Joback Method
tc	771.41	K	Joback Method
tf	335.16	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.26	J/mol×K	613.47	Joback Method
cpg	663.52	J/mol×K	639.79	Joback Method

cpg	679.08	J/mol×K	666.12	Joback Method
cpg	693.94	J/mol×K	692.44	Joback Method
cpg	708.13	J/mol×K	718.76	Joback Method
cpg	721.67	J/mol×K	745.09	Joback Method
cpg	734.58	J/mol×K	771.41	Joback Method

Sources

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=C53800025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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