Undecyl trifluoroacetate

Other names: Trifluoroacetic acid, undecyl ester
Inchi: InChI=1S/C13H23F3O2/c1-2-3-4-5-6-7-8-9-10-11-18-12(17)13(14,15)16/h2-11H2,1H3
InchiKey: OSMPYUQBJFIJED-UHFFFAOYSA-N
Formula: C13H23F3O2
SMILES: CCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 268.32

Physical Properties

Property code	Value	Unit	Source
af	0.7003		Cheméo Relay (1.0)
hf	-1206.14	kJ/mol	Cheméo Relay (1.0)
hfus	34.04	kJ/mol	Joback Method
hvap	68.55	kJ/mol	Cheméo Relay (1.0)
ie	10.47	eV	Cheméo Relay (1.0)
log10ws	-4.82		Cheméo Relay (1.0)
logp	4.623		Crippen Method
mcvol	206.780	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1343.60		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1343.60		NIST Webbook
tb	491.63	K	Cheméo Relay (1.0)
tc	615.40	K	Cheméo Relay (1.0)
tf	254.95	K	Cheméo Relay (1.0)
vc	0.794	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.88	J/mol×K	567.71	Joback Method
cpg	557.10	J/mol×K	593.97	Joback Method
cpg	571.66	J/mol×K	620.24	Joback Method
cpg	585.58	J/mol×K	646.50	Joback Method

cpg	598.89	J/mol×K	672.77	Joback Method
cpg	611.59	J/mol×K	699.03	Joback Method
cpg	623.71	J/mol×K	725.30	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C53800014&Units=SI

Legend

af:	Acentric Factor
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume