

Acetic acid, trifluoro-, undecyl ester

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:	OSMPYUQBFIJED-UHFFFAOYSA-N
Formula:	C13H23F3O2
SMILES:	CCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	268.32
CAS:	53800-01-4

Physical Properties

Property code	Value	Unit	Source
gf	-756.93	kJ/mol	Joback Method
hf	-1153.53	kJ/mol	Joback Method
hfus	34.04	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.623		Crippen Method
mcvol	206.780	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1343.60		NIST Webbook
rinpol	1343.60		NIST Webbook
tb	567.71	K	Joback Method
tc	725.30	K	Joback Method
tf	312.62	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53800014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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