

2-(Nonyloxy)ethanol, TFA

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H23F3O3/c1-2-3-4-5-6-7-8-9-18-10-11-19-12(17)13(14,15)16/h2-11H2,1H3

HJVRJJLSUMFICM-UHFFFAOYSA-N

C13H23F3O3

CCCCCCCCCOCCOC(=O)C(F)(F)F

284.32

Physical Properties

Property code	Value	Unit	Source
gf	-861.93	kJ/mol	Joback Method
hf	-1285.75	kJ/mol	Joback Method
hfus	35.23	kJ/mol	Joback Method
hvap	52.35	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.859		Crippen Method
mcvol	212.650	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1444.80		NIST Webbook
tb	590.13	K	Joback Method
tc	748.28	K	Joback Method
tf	334.85	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.51	J/mol×K	590.13	Joback Method
cpg	585.50	J/mol×K	616.49	Joback Method
cpg	599.87	J/mol×K	642.85	Joback Method
cpg	613.61	J/mol×K	669.20	Joback Method
cpg	626.75	J/mol×K	695.56	Joback Method
cpg	639.29	J/mol×K	721.92	Joback Method
cpg	651.26	J/mol×K	748.28	Joback Method

Sources

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=R184491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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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