

2-(2-(2-(2-nonyloxy-ethoxy)-ethoxy)-ethoxy)-ethanol

TFA
InchiKey:

InChI=1S/C19H35F3O6/c1-2-3-4-5-6-7-8-9-24-10-11-25-12-13-26-14-15-27-16-17-28-18

Formula:

C19H35F3O6

SMILES:

CCCCCCCCCOCCOCCOCCOCCOC(=O)C(F)(F)F

Mol. weight [g/mol]:

416.47

Physical Properties

Property code	Value	Unit	Source
gf	-1126.41	kJ/mol	Joback Method
hf	-1806.25	kJ/mol	Joback Method
hfus	54.33	kJ/mol	Joback Method
hvap	72.94	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.909		Crippen Method
mcvol	314.800	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2229.80		NIST Webbook
tb	794.67	K	Joback Method
tc	972.92	K	Joback Method
tf	469.16	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.78	J/molxK	794.67	Joback Method
cpg	1019.69	J/molxK	824.38	Joback Method
cpg	1036.52	J/molxK	854.09	Joback Method
cpg	1052.28	J/molxK	883.79	Joback Method
cpg	1066.98	J/molxK	913.50	Joback Method
cpg	1080.62	J/molxK	943.21	Joback Method
cpg	1093.20	J/molxK	972.92	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=R184268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
mccol:	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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