

2-(2-(2-decyloxy-ethoxy)-ethoxy)-ethanol, TFA

Inchi:	InChI=1S/C18H33F3O5/c1-2-3-4-5-6-7-8-9-10-23-11-12-24-13-14-25-15-16-26-17(22)18
InchiKey:	WBCHIXGHBBOLBU-UHFFFAOYSA-N
Formula:	C18H33F3O5
SMILES:	CCCCCCCCCOCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	386.45

Physical Properties

Property code	Value	Unit	Source
gf	-1029.83	kJ/mol	Joback Method
hf	-1653.39	kJ/mol	Joback Method
hfus	50.55	kJ/mol	Joback Method
hvap	68.30	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	4.282		Crippen Method
mvol	294.840	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	2067.80		NIST Webbook
rinpol	2067.80		NIST Webbook
tb	749.37	K	Joback Method
tc	919.21	K	Joback Method
tf	435.66	K	Joback Method
vc	1.165	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.27	J/molxK	749.37	Joback Method
cpg	927.69	J/molxK	777.68	Joback Method
cpg	944.20	J/molxK	805.98	Joback Method
cpg	959.82	J/molxK	834.29	Joback Method
cpg	974.54	J/molxK	862.60	Joback Method
cpg	988.39	J/molxK	890.91	Joback Method
cpg	1001.36	J/molxK	919.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184302&Units=SI

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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