

2-(2-(2-(2-Pentoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy

trifluoroacetate

InChIKey:

InChI=1S/C17H31F3O7/c1-2-3-4-5-22-6-7-23-8-9-24-10-11-25-12-13-26-14-15-27-16(21

RRZLWMXLRMOERJ-UHFFFAOYSA-N

Formula:

C17H31F3O7

SMILES:

CCCCOCCOCCOCCOCCOCCOC(=O)C(F)(F)F

Mol. weight [g/mol]:

404.42

Physical Properties

Property code	Value	Unit	Source
gf	-1248.25	kJ/mol	Joback Method
hf	-1897.19	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	2.365		Crippen Method
mvol	292.490	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	2102.50		NIST Webbook
tb	771.33	K	Joback Method
tc	945.05	K	Joback Method
tf	468.85	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.68	J/molxK	771.33	Joback Method
cpg	930.42	J/molxK	800.28	Joback Method
cpg	946.19	J/molxK	829.24	Joback Method
cpg	960.98	J/molxK	858.19	Joback Method
cpg	974.79	J/molxK	887.14	Joback Method
cpg	987.61	J/molxK	916.09	Joback Method
cpg	999.43	J/molxK	945.05	Joback Method

Sources

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=R188379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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