2-(2-(2-(2-(2-(2-decyloxy-ethoxy)-ethoxy)-ethoxy)-e TFA

Inchi: InChI=1S/C24H45F3O8/c1-2-3-4-5-6-7-8-9-10-29-11-12-30-13-14-31-15-16-32-17-18-33
InchiKey: WVCOKZMBNLWPHL-UHFFFAOYSA-N
Formula: C24H45F3O8
SMILES: CCCCCCCCCCOCCOCCOCCOCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 518.60

Physical Properties

Property code	Value	Unit	Source
gf	-1294.31	kJ/mol	Joback Method
hf	-2173.89	kJ/mol	Joback Method
hfus	69.66	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	4.332		Crippen Method
mcvol	396.990	ml/mol	McGowan Method
pc	732.84	kPa	Joback Method
rinpol	2862.70		NIST Webbook
tb	953.91	K	Joback Method
tc	1190.30	K	Joback Method
tf	569.97	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1375.28	J/mol×K	953.91	Joback Method
cpg	1395.52	J/mol×K	993.31	Joback Method
cpg	1413.29	J/mol×K	1032.71	Joback Method
cpg	1428.58	J/mol×K	1072.10	Joback Method
cpg	1441.38	J/mol×K	1111.50	Joback Method
cpg	1451.68	J/mol×K	1150.90	Joback Method
cpg	1459.47	J/mol×K	1190.30	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=R184060&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
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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