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

Inchi: InChI=1S/C16H29F3O4/c1-2-3-4-5-6-7-8-9-10-21-11-12-22-13-14-23-15(20)16(17,18)19
InchiKey: ADQUVHVEPVEJTQ-UHFFFAOYSA-N
Formula: C16H29F3O4
SMILES: CCCCCCCCCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 342.39

Physical Properties

Property code	Value	Unit	Source
gf	-941.67	kJ/mol	Joback Method
hf	-1479.89	kJ/mol	Joback Method
hfus	44.19	kJ/mol	Joback Method
hvap	61.44	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.266		Crippen Method
mcvol	260.790	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	1804.30		NIST Webbook
tb	681.19	K	Joback Method
tc	843.15	K	Joback Method
tf	390.89	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.26	J/mol×K	681.19	Joback Method
cpg	779.71	J/mol×K	708.18	Joback Method
cpg	795.42	J/mol×K	735.18	Joback Method
cpg	810.38	J/mol×K	762.17	Joback Method
cpg	824.61	J/mol×K	789.16	Joback Method
cpg	838.13	J/mol×K	816.15	Joback Method
cpg	850.94	J/mol×K	843.15	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=R184382&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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