2-decyloxy-ethanol, TFA

Inchi: InChI=1S/C14H25F3O3/c1-2-3-4-5-6-7-8-9-10-19-11-12-20-13(18)14(15,16)17/h2-12H2,
InchiKey: WQVGLULVVLMLBG-UHFFFAOYSA-N
Formula: C14H25F3O3
SMILES: CCCCCCCCCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 298.34

Physical Properties

Property code	Value	Unit	Source
gf	-853.51	kJ/mol	Joback Method
hf	-1306.39	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.249		Crippen Method
mcvol	226.740	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
tb	613.01	K	Joback Method
tc	771.44	K	Joback Method
tf	346.12	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.19	J/mol×K	613.01	Joback Method
cpg	638.74	J/mol×K	639.41	Joback Method
cpg	653.62	J/mol×K	665.82	Joback Method
cpg	667.85	J/mol×K	692.22	Joback Method
cpg	681.44	J/mol×K	718.63	Joback Method
cpg	694.41	J/mol×K	745.03	Joback Method
cpg	706.77	J/mol×K	771.44	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=R184466&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