9-Decen-1-ol, trifluoroacetate

Inchi: InChI=1S/C12H19F3O2/c1-2-3-4-5-6-7-8-9-10-17-11(16)12(13,14)15/h2H,1,3-10H2
InchiKey: KKLWRPBVKFLPBB-UHFFFAOYSA-N
Formula: C12H19F3O2
SMILES: C=CCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 252.27

Physical Properties

Property code	Value	Unit	Source
gf	-677.51	kJ/mol	Joback Method
hf	-1007.46	kJ/mol	Joback Method
hfus	30.17	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.009		Crippen Method
mcvol	188.390	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1252.70		NIST Webbook
rinpol	1252.70		NIST Webbook
tb	541.51	K	Joback Method
tc	701.68	K	Joback Method
tf	299.59	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.78	J/mol×K	541.51	Joback Method
cpg	485.92	J/mol×K	568.20	Joback Method
cpg	499.42	J/mol×K	594.90	Joback Method
cpg	512.31	J/mol×K	621.59	Joback Method
cpg	524.59	J/mol×K	648.29	Joback Method
cpg	536.31	J/mol×K	674.98	Joback Method
cpg	547.46	J/mol×K	701.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352659&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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