1-Octen-3-ol, trifluoroacetate

Inchi: InChI=1S/C10H15F3O2/c1-3-5-6-7-8(4-2)15-9(14)10(11,12)13/h4,8H,2-3,5-7H2,1H3
InchiKey: WAFGKSJTIVSIER-UHFFFAOYSA-N
Formula: C10H15F3O2
SMILES: C=CC(CCCCC)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 224.22

Physical Properties

Property code	Value	Unit	Source
gf	-696.79	kJ/mol	Joback Method
hf	-971.46	kJ/mol	Joback Method
hfus	21.47	kJ/mol	Joback Method
hvap	42.20	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.227		Crippen Method
mcvol	160.210	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	951.40		NIST Webbook
rinpol	951.40		NIST Webbook
tb	495.31	K	Joback Method
tc	659.93	K	Joback Method
tf	262.05	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.66	J/mol×K	495.31	Joback Method
cpg	390.74	J/mol×K	522.75	Joback Method
cpg	403.22	J/mol×K	550.18	Joback Method
cpg	415.11	J/mol×K	577.62	Joback Method
cpg	426.43	J/mol×K	605.06	Joback Method
cpg	437.20	J/mol×K	632.49	Joback Method
cpg	447.43	J/mol×K	659.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352755&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