Acetic acid, trifluoro, 1-methylheptyl ester

Inchi: InChI=1S/C10H17F3O2/c1-3-4-5-6-7-8(2)15-9(14)10(11,12)13/h8H,3-7H2,1-2H3
InchiKey: OSUSEXASYGZJOJ-UHFFFAOYSA-N
Formula: C10H17F3O2
SMILES: CCCCCCC(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 226.24
CAS: 332-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-784.63	kJ/mol	Joback Method
hf	-1096.89	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	42.88	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.451		Crippen Method
mcvol	164.510	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	967.00		NIST Webbook
rinpol	991.50		NIST Webbook
rinpol	991.50		NIST Webbook
rinpol	967.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1075.00		NIST Webbook
tb	498.63	K	Joback Method
tc	660.43	K	Joback Method
tf	263.81	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.78	J/mol×K	498.63	Joback Method
cpg	409.38	J/mol×K	525.60	Joback Method
cpg	422.39	J/mol×K	552.56	Joback Method

cpg	434.81	J/mol×K	579.53	Joback Method
cpg	446.68	J/mol×K	606.50	Joback Method
cpg	458.01	J/mol×K	633.47	Joback Method
cpg	468.80	J/mol×K	660.43	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C332832&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume