3-Methyl-3-pentanol, trifluoroacetate

Inchi: InChI=1S/C8H13F3O2/c1-4-7(3,5-2)13-6(12)8(9,10)11/h4-5H2,1-3H3
InchiKey: XSMKVYXJBIUWMI-UHFFFAOYSA-N
Formula: C8H13F3O2
SMILES: CCC(C)(CC)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 198.18

Physical Properties

Property code	Value	Unit	Source
gf	-796.19	kJ/mol	Joback Method
hf	-1059.08	kJ/mol	Joback Method
hfus	13.67	kJ/mol	Joback Method
hvap	37.52	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.671		Crippen Method
mcvol	136.330	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	793.00		NIST Webbook
rinpol	793.00		NIST Webbook
tb	450.08	K	Joback Method
tc	619.72	K	Joback Method
tf	258.69	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.57	J/mol×K	450.08	Joback Method
cpg	322.30	J/mol×K	478.35	Joback Method
cpg	334.37	J/mol×K	506.63	Joback Method
cpg	345.80	J/mol×K	534.90	Joback Method
cpg	356.62	J/mol×K	563.17	Joback Method
cpg	366.84	J/mol×K	591.45	Joback Method
cpg	376.50	J/mol×K	619.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375652&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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