2,4-Dimethyl-3-pentanol, trifluoroacetate

Inchi: InChI=1S/C9H15F3O2/c1-5(2)7(6(3)4)14-8(13)9(10,11)12/h5-7H,1-4H3
InchiKey: WOVKJHJBPIFBJG-UHFFFAOYSA-N
Formula: C9H15F3O2
SMILES: CC(C)C(OC(=O)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 212.21

Physical Properties

Property code	Value	Unit	Source
gf	-797.93	kJ/mol	Joback Method
hf	-1086.81	kJ/mol	Joback Method
hfus	13.11	kJ/mol	Joback Method
hvap	39.87	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.772		Crippen Method
mcvol	150.420	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	835.00		NIST Webbook
tb	474.87	K	Joback Method
tc	644.13	K	Joback Method
tf	222.54	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.80	J/mol×K	474.87	Joback Method
cpg	364.28	J/mol×K	503.08	Joback Method
cpg	377.15	J/mol×K	531.29	Joback Method
cpg	389.42	J/mol×K	559.50	Joback Method
cpg	401.10	J/mol×K	587.71	Joback Method
cpg	412.22	J/mol×K	615.92	Joback Method
cpg	422.79	J/mol×K	644.13	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=U375657&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