2-Methyl-1-pentanol, pentafluoropropionate

Inchi: InChI=1S/C9H13F5O2/c1-3-4-6(2)5-16-7(15)8(10,11)9(12,13)14/h6H,3-5H2,1-2H3
InchiKey: JEIWISMWHQVTKH-UHFFFAOYSA-N
Formula: C9H13F5O2
SMILES: CCCC(C)COC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 248.19

Physical Properties

Property code	Value	Unit	Source
gf	-1179.83	kJ/mol	Joback Method
hf	-1477.22	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.163		Crippen Method
mcvol	153.960	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	838.50		NIST Webbook
rinpol	838.50		NIST Webbook
tb	471.06	K	Joback Method
tc	627.66	K	Joback Method
tf	256.14	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.62	J/mol×K	471.06	Joback Method
cpg	382.31	J/mol×K	497.16	Joback Method
cpg	394.39	J/mol×K	523.26	Joback Method
cpg	405.85	J/mol×K	549.36	Joback Method
cpg	416.73	J/mol×K	575.46	Joback Method
cpg	427.04	J/mol×K	601.56	Joback Method
cpg	436.81	J/mol×K	627.66	Joback Method

Sources

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=U352359&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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