2-Pentanol, trifluoroacetate

Inchi: InChI=1S/C7H11F3O2/c1-3-4-5(2)12-6(11)7(8,9)10/h5H,3-4H2,1-2H3
InchiKey: HENNKZFOVKJQDI-UHFFFAOYSA-N
Formula: C7H11F3O2
SMILES: CCCC(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 184.16
CAS: 90991-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-809.89	kJ/mol	Joback Method
hf	-1034.97	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	36.20	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.280		Crippen Method
mcvol	122.240	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	747.50		NIST Webbook
rinpol	747.50		NIST Webbook
tb	429.99	K	Joback Method
tc	594.24	K	Joback Method
tf	230.00	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.92	J/mol×K	429.99	Joback Method
cpg	276.90	J/mol×K	457.36	Joback Method
cpg	287.40	J/mol×K	484.74	Joback Method
cpg	297.44	J/mol×K	512.11	Joback Method
cpg	307.02	J/mol×K	539.49	Joback Method
cpg	316.16	J/mol×K	566.86	Joback Method
cpg	324.86	J/mol×K	594.24	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=C90991712&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

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