3-Heptanol, trifluoroacetate

Inchi: InChI=1S/C9H15F3O2/c1-3-5-6-7(4-2)14-8(13)9(10,11)12/h7H,3-6H2,1-2H3
InchiKey: ISBQSSHMLYEHKL-UHFFFAOYSA-N
Formula: C9H15F3O2
SMILES: CCCCC(CC)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 212.21
CAS: 90991-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-793.05	kJ/mol	Joback Method
hf	-1076.25	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	40.65	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.061		Crippen Method
mcvol	150.420	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
tb	475.75	K	Joback Method
tc	638.38	K	Joback Method
tf	252.54	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.52	J/mol×K	475.75	Joback Method
cpg	363.33	J/mol×K	502.85	Joback Method
cpg	375.59	J/mol×K	529.96	Joback Method
cpg	387.31	J/mol×K	557.06	Joback Method
cpg	398.50	J/mol×K	584.17	Joback Method
cpg	409.17	J/mol×K	611.27	Joback Method
cpg	419.35	J/mol×K	638.38	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=C90991698&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