3-Hexyltrifluoroacetate

Inchi: InChI=1S/C8H13F3O2/c1-3-5-6(4-2)13-7(12)8(9,10)11/h6H,3-5H2,1-2H3
InchiKey: TXLRKFWFZMQEOY-UHFFFAOYSA-N
Formula: C8H13F3O2
SMILES: CCCC(CC)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 198.18
CAS: 761-34-2

Physical Properties

Property code	Value	Unit	Source
gf	-801.47	kJ/mol	Joback Method
hf	-1055.61	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	38.42	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.671		Crippen Method
mcvol	136.330	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	796.40		NIST Webbook
tb	452.87	K	Joback Method
tc	616.33	K	Joback Method
tf	241.27	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.19	J/mol×K	452.87	Joback Method
cpg	319.14	J/mol×K	480.11	Joback Method
cpg	330.57	J/mol×K	507.36	Joback Method
cpg	341.49	J/mol×K	534.60	Joback Method
cpg	351.92	J/mol×K	561.85	Joback Method
cpg	361.87	J/mol×K	589.09	Joback Method
cpg	371.35	J/mol×K	616.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C761342&Units=SI

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