Hexyl trifluoroacetate

Other names:	Hexyl 2,2,2-trifluoroacetate
	1-Hexanol, trifluoroacetate
	Trifluoroacetic acid, n-hexyl ester
	Acetic acid, trifluoro-, hexyl ester
	Trifluoroacetic acid, hexyl ester
Inchi:	InChI=1S/C8H13F3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h2-6H2,1H3
InchiKey:	DTTIQEHOYLOWDU-UHFFFAOYSA-N
Formula:	C8H13F3O2
SMILES:	CCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	198.18
CAS:	400-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-799.03	kJ/mol	Joback Method
hf	-1050.33	kJ/mol	Joback Method
hfus	21.09	kJ/mol	Joback Method
hvap	38.81	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.672		Crippen Method
mcvol	136.330	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	858.80		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	867.10		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	830.80		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	851.50		NIST Webbook
rinpol	852.00		NIST Webbook
ripol	980.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	980.00		NIST Webbook
tb	453.31	K	Joback Method
tc	613.49	K	Joback Method

tf	256.27	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.09	J/mol×K	453.31	Joback Method
cpg	318.73	J/mol×K	480.01	Joback Method
cpg	329.87	J/mol×K	506.70	Joback Method
cpg	340.53	J/mol×K	533.40	Joback Method
cpg	350.72	J/mol×K	560.09	Joback Method
cpg	360.46	J/mol×K	586.79	Joback Method
cpg	369.75	J/mol×K	613.49	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=C400613&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
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume