Ether, octyl 2,2,2-trifluoro-1-methylethyl, (±)-

Inchi: InChI=1S/C11H21F3O/c1-3-4-5-6-7-8-9-15-10(2)11(12,13)14/h10H,3-9H2,1-2H3
InchiKey: UBUIQVZDLONGTK-UHFFFAOYSA-N
Formula: C11H21F3O
SMILES: CCCCCCCCOC(C)C(F)(F)F
Mol. weight [g/mol]: 226.28
CAS: 3540-04-3

Physical Properties

Property code	Value	Unit	Source
gf	-647.29	kJ/mol	Joback Method
hf	-1004.95	kJ/mol	Joback Method
hfus	23.74	kJ/mol	Joback Method
hvap	38.36	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.314		Crippen Method
mcvol	177.030	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
tb	467.64	K	Joback Method
tc	619.47	K	Joback Method
tf	225.15	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.82	J/mol×K	467.64	Joback Method
cpg	429.95	J/mol×K	492.94	Joback Method
cpg	444.49	J/mol×K	518.25	Joback Method
cpg	458.46	J/mol×K	543.55	Joback Method
cpg	471.86	J/mol×K	568.86	Joback Method
cpg	484.72	J/mol×K	594.16	Joback Method
cpg	497.05	J/mol×K	619.47	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=C3540043&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume