Heneicosyl trifluoroacetate

Other names: Heneicosyl 2,2,2-trifluoroacetate
1-Heneicosanol, trifluoroacetate
Inchi: InChI=1S/C23H43F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-28-22
InchiKey: YAOMXMSGWKCKPX-UHFFFAOYSA-N
Formula: C23H43F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 408.58

Physical Properties

Property code	Value	Unit	Source
gf	-672.73	kJ/mol	Joback Method
hf	-1359.93	kJ/mol	Joback Method
hfus	59.94	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.524		Crippen Method
mcvol	347.680	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
tb	796.51	K	Joback Method
tc	975.17	K	Joback Method
tf	425.32	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.40	J/mol×K	796.51	Joback Method
cpg	1136.84	J/mol×K	826.29	Joback Method
cpg	1156.21	J/mol×K	856.06	Joback Method
cpg	1174.55	J/mol×K	885.84	Joback Method
cpg	1191.90	J/mol×K	915.62	Joback Method
cpg	1208.31	J/mol×K	945.40	Joback Method
cpg	1223.83	J/mol×K	975.17	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=U351765&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume