«alpha»-Hydroxynervonic acid, HFB-Me

Inchi: InChI=1S/C29H47F7O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-2
InchiKey: JNINHMOSIJZDCZ-MSUUIHNZSA-N
Formula: C29H47F7O4
SMILES: CCCCCCCCCCCCCCC=CCCCCCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)OC
Mol. weight [g/mol]: 592.67

Physical Properties

Property code	Value	Unit	Source
gf	-1551.91	kJ/mol	Joback Method
hf	-2418.57	kJ/mol	Joback Method
hfus	72.44	kJ/mol	Joback Method
hvap	88.42	kJ/mol	Joback Method
log10ws	-10.94		Crippen Method
logp	9.892		Crippen Method
mcvol	442.440	ml/mol	McGowan Method
pc	592.57	kPa	Joback Method
rinpol	2725.00		NIST Webbook
tb	1004.42	K	Joback Method
tc	1266.66	K	Joback Method
tf	552.22	K	Joback Method
vc	1.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1556.84	J/mol×K	1004.42	Joback Method
cpg	1580.39	J/mol×K	1048.13	Joback Method
cpg	1602.36	J/mol×K	1091.83	Joback Method
cpg	1623.00	J/mol×K	1135.54	Joback Method
cpg	1642.57	J/mol×K	1179.25	Joback Method
cpg	1661.32	J/mol×K	1222.95	Joback Method
cpg	1679.51	J/mol×K	1266.66	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=R134302&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