

«alpha»-Hydroxylignoceric acid, HFB-Me

Inchi:	InChI=1S/C29H49F7O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-2
InchiKey:	QRJUMVCTBZKGFE-UHFFFAOYSA-N
Formula:	C29H49F7O4
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)OC
Mol. weight [g/mol]:	594.69

Physical Properties

Property code	Value	Unit	Source
gf	-1632.13	kJ/mol	Joback Method
hf	-2535.79	kJ/mol	Joback Method
hfus	72.23	kJ/mol	Joback Method
hvap	88.47	kJ/mol	Joback Method
log10ws	-11.09		Crippen Method
logp	10.116		Crippen Method
mcvol	446.740	ml/mol	McGowan Method
pc	577.85	kPa	Joback Method
rinsol	2753.00		NIST Webbook
tb	1000.26	K	Joback Method
tc	1267.57	K	Joback Method
tf	557.30	K	Joback Method
vc	1.794	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.09	J/mol×K	1000.26	Joback Method
cpg	1609.37	J/mol×K	1044.81	Joback Method
cpg	1631.72	J/mol×K	1089.36	Joback Method
cpg	1652.40	J/mol×K	1133.91	Joback Method
cpg	1671.65	J/mol×K	1178.47	Joback Method
cpg	1689.70	J/mol×K	1223.02	Joback Method
cpg	1706.82	J/mol×K	1267.57	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=R134288&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
mccvol:	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

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