

«alpha»-Hydroxystearic acid, HFB-Me

Inchi:	InChI=1S/C23H37F7O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19(31)33-2)34-20
InchiKey:	KEYQLGZMFHOTEW-UHFFFAOYSA-N
Formula:	C23H37F7O4
SMILES:	CCCCCCCCCCCCCCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)OC
Mol. weight [g/mol]:	510.53

Physical Properties

Property code	Value	Unit	Source
gf	-1682.65	kJ/mol	Joback Method
hf	-2411.95	kJ/mol	Joback Method
hfus	56.69	kJ/mol	Joback Method
hvap	75.11	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	7.776		Crippen Method
mvol	362.200	ml/mol	McGowan Method
pc	778.51	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	862.98	K	Joback Method
tc	1060.18	K	Joback Method
tf	489.68	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.35	J/mol×K	862.98	Joback Method
cpg	1224.71	J/mol×K	895.85	Joback Method
cpg	1241.88	J/mol×K	928.71	Joback Method
cpg	1257.93	J/mol×K	961.58	Joback Method
cpg	1272.95	J/mol×K	994.44	Joback Method
cpg	1287.02	J/mol×K	1027.31	Joback Method
cpg	1300.22	J/mol×K	1060.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=R134362&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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