

«alpha»-Hydroxytricosanoic acid, HFB-Me

Inchi:	InChI=1S/C28H47F7O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(2
InchiKey:	GBFVMFJLGCUPOZ-UHFFFAOYSA-N
Formula:	C28H47F7O4
SMILES:	CCCCCCCCCCCCCCCCCCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)OC
Mol. weight [g/mol]:	580.66

Physical Properties

Property code	Value	Unit	Source
gf	-1640.55	kJ/mol	Joback Method
hf	-2515.15	kJ/mol	Joback Method
hfus	69.64	kJ/mol	Joback Method
hvap	86.24	kJ/mol	Joback Method
log10ws	-10.67		Crippen Method
logp	9.726		Crippen Method
mcvol	432.650	ml/mol	McGowan Method
pc	605.47	kPa	Joback Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook
tb	977.38	K	Joback Method
tc	1229.33	K	Joback Method
tf	546.03	K	Joback Method
vc	1.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.71	J/mol×K	977.38	Joback Method
cpg	1543.75	J/mol×K	1019.37	Joback Method
cpg	1565.02	J/mol×K	1061.36	Joback Method
cpg	1584.72	J/mol×K	1103.36	Joback Method
cpg	1603.05	J/mol×K	1145.35	Joback Method
cpg	1620.21	J/mol×K	1187.34	Joback Method
cpg	1636.41	J/mol×K	1229.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R134382&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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