

«alpha»-Hydroxyarachidic acid, HFB-Me

Inchi:	InChI=1S/C25H41F7O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21(33)35-2
InchiKey:	KJVXKRLFFXIGKP-UHFFFAOYSA-N
Formula:	C25H41F7O4
SMILES:	CCCCCCCCCCCCCCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)OC
Mol. weight [g/mol]:	538.58

Physical Properties

Property code	Value	Unit	Source
gf	-1665.81	kJ/mol	Joback Method
hf	-2453.23	kJ/mol	Joback Method
hfus	61.87	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	8.556		Crippen Method
mcvol	390.380	ml/mol	McGowan Method
pc	701.35	kPa	Joback Method
rinpol	2374.00		NIST Webbook
tb	908.74	K	Joback Method
tc	1123.90	K	Joback Method
tf	512.22	K	Joback Method
vc	1.571	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1330.44	J/mol×K	908.74	Joback Method
cpg	1350.41	J/mol×K	944.60	Joback Method
cpg	1368.99	J/mol×K	980.46	Joback Method
cpg	1386.30	J/mol×K	1016.32	Joback Method
cpg	1402.45	J/mol×K	1052.18	Joback Method
cpg	1417.55	J/mol×K	1088.04	Joback Method
cpg	1431.72	J/mol×K	1123.90	Joback Method

Sources

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=R134208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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