1-(4-Hydroxy-3-methoxyphenyl)hexadecane-3,5-d

Other names: [12]-Gingerdione
Inchi: InChI=1S/C23H36O4/c1-3-4-5-6-7-8-9-10-11-12-20(24)18-21(25)15-13-19-14-16-22(26)2
InchiKey: SRGFWRMSKPVJOD-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCCCCC(=O)CC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 376.53
CAS: 91815-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-271.90	kJ/mol	Joback Method
hf	-827.68	kJ/mol	Joback Method
hfus	59.15	kJ/mol	Joback Method
hvap	98.65	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.783		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	2995.80		NIST Webbook
rinpol	2995.80		NIST Webbook
tb	968.08	K	Joback Method
tc	1186.06	K	Joback Method
tf	621.72	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.39	J/mol×K	968.08	Joback Method
cpg	1165.40	J/mol×K	1149.73	Joback Method
cpg	1151.34	J/mol×K	1113.40	Joback Method
cpg	1136.71	J/mol×K	1077.07	Joback Method
cpg	1121.40	J/mol×K	1040.74	Joback Method
cpg	1105.32	J/mol×K	1004.41	Joback Method

cpg	1178.97	J/mol×K	1186.06	Joback Method
dvisc	0.0000017	Pa×s	968.08	Joback Method
dvisc	0.0000024	Pa×s	910.35	Joback Method
dvisc	0.0000037	Pa×s	852.63	Joback Method
dvisc	0.0000059	Pa×s	794.90	Joback Method
dvisc	0.0000102	Pa×s	737.17	Joback Method
dvisc	0.0000195	Pa×s	679.45	Joback Method
dvisc	0.0000418	Pa×s	621.72	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91815315&Units=SI
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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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