1-(4-Hydroxy-3-methoxyphenyl)tetradecan-3-one

Inchi: InChI=1S/C21H34O3/c1-3-4-5-6-7-8-9-10-11-12-19(22)15-13-18-14-16-20(23)21(17-18)2
InchiKey: XNBUKRQGYHYOOP-UHFFFAOYSA-N
Formula: C21H34O3
SMILES: CCCCCCCCCCCC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 334.49
CAS: 36700-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-159.82	kJ/mol	Joback Method
hf	-673.82	kJ/mol	Joback Method
hfus	52.37	kJ/mol	Joback Method
hvap	87.45	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.823		Crippen Method
mcvol	296.300	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2669.80		NIST Webbook
tb	868.45	K	Joback Method
tc	1071.88	K	Joback Method
tf	549.25	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.84	J/mol×K	868.45	Joback Method
cpg	966.07	J/mol×K	902.35	Joback Method
cpg	982.43	J/mol×K	936.26	Joback Method
cpg	998.00	J/mol×K	970.16	Joback Method
cpg	1012.86	J/mol×K	1004.07	Joback Method
cpg	1027.07	J/mol×K	1037.97	Joback Method
cpg	1040.72	J/mol×K	1071.88	Joback Method
dvisc	0.0000954	Pa×s	549.25	Joback Method

dvisc	0.0000417	Pa×s	602.45	Joback Method
dvisc	0.0000208	Pa×s	655.65	Joback Method
dvisc	0.0000116	Pa×s	708.85	Joback Method
dvisc	0.0000070	Pa×s	762.05	Joback Method
dvisc	0.0000045	Pa×s	815.25	Joback Method
dvisc	0.0000030	Pa×s	868.45	Joback Method

Sources

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=C36700488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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