

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.84	J/molxK	868.45	Joback Method
cpg	1027.07	J/molxK	1037.97	Joback Method
cpg	1012.86	J/molxK	1004.07	Joback Method
cpg	998.00	J/molxK	970.16	Joback Method
cpg	982.43	J/molxK	936.26	Joback Method
cpg	966.07	J/molxK	902.35	Joback Method
cpg	1040.72	J/molxK	1071.88	Joback Method
dvisc	0.0000030	Paxs	868.45	Joback Method

dvisc	0.0000045	Paxs	815.25	Joback Method
dvisc	0.0000070	Paxs	762.05	Joback Method
dvisc	0.0000116	Paxs	708.85	Joback Method
dvisc	0.0000208	Paxs	655.65	Joback Method
dvisc	0.0000417	Paxs	602.45	Joback Method
dvisc	0.0000954	Paxs	549.25	Joback Method

Sources

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/80-256-9/1-4-Hydroxy-3-methoxyphenyl-tetradecan-3-one.pdf>

Generated by Cheméo on 2024-04-27 06:54:50.55264521 +0000 UTC m=+16490139.473222574.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.