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

Inchi: InChI=1S/C19H30O3/c1-3-4-5-6-7-8-9-10-17(20)13-11-16-12-14-18(21)19(15-16)22-2/h1
InchiKey: TYQRTQZWHUXDLG-UHFFFAOYSA-N
Formula: C19H30O3
SMILES: CCCCCCCCCC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 306.44
CAS: 27113-23-1

Physical Properties

Property code	Value	Unit	Source
gf	-176.66	kJ/mol	Joback Method
hf	-632.54	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	5.043		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2459.10		NIST Webbook
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
rinpol	2459.10		NIST Webbook
tb	822.69	K	Joback Method
tc	1024.97	K	Joback Method
tf	526.71	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.00	J/mol×K	822.69	Joback Method
cpg	846.45	J/mol×K	856.40	Joback Method
cpg	862.07	J/mol×K	890.12	Joback Method
cpg	876.91	J/mol×K	923.83	Joback Method
cpg	891.04	J/mol×K	957.55	Joback Method

cpg	904.53	J/mol×K	991.26	Joback Method
cpg	917.44	J/mol×K	1024.97	Joback Method
dvisc	0.0001360	Pa×s	526.71	Joback Method
dvisc	0.0000607	Pa×s	576.04	Joback Method
dvisc	0.0000308	Pa×s	625.37	Joback Method
dvisc	0.0000172	Pa×s	674.70	Joback Method
dvisc	0.0000104	Pa×s	724.03	Joback Method
dvisc	0.0000067	Pa×s	773.36	Joback Method
dvisc	0.0000046	Pa×s	822.69	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=C27113231&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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