1-(4-Hydroxy-3-methoxyphenyl)dodec-1-ene-3,5-d

Inchi: InChI=1S/C19H26O4/c1-3-4-5-6-7-8-16(20)14-17(21)11-9-15-10-12-18(22)19(13-15)23-2
InchiKey: QOJHXMDTWFYFRL-PKNBQFBNSA-N
Formula: C19H26O4
SMILES: CCCCCCCC(=O)CC(=O)C=Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 318.41
CAS: 748159-34-4

Physical Properties

Property code	Value	Unit	Source
gf	-225.36	kJ/mol	Joback Method
hf	-627.90	kJ/mol	Joback Method
hfus	48.99	kJ/mol	Joback Method
hvap	89.70	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.303		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2823.60		NIST Webbook
tb	880.72	K	Joback Method
tc	1095.04	K	Joback Method
tf	571.56	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.64	J/mol×K	880.72	Joback Method
cpg	834.41	J/mol×K	916.44	Joback Method
cpg	848.48	J/mol×K	952.16	Joback Method
cpg	861.93	J/mol×K	987.88	Joback Method
cpg	874.85	J/mol×K	1023.60	Joback Method
cpg	887.32	J/mol×K	1059.32	Joback Method
cpg	899.44	J/mol×K	1095.04	Joback Method
dvisc	0.0000786	Pa×s	571.56	Joback Method

dvisc	0.0000371	Pa×s	623.09	Joback Method
dvisc	0.0000196	Pa×s	674.61	Joback Method
dvisc	0.0000114	Pa×s	726.14	Joback Method
dvisc	0.0000071	Pa×s	777.67	Joback Method
dvisc	0.0000047	Pa×s	829.19	Joback Method
dvisc	0.0000033	Pa×s	880.72	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=C748159344&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