1-(4-Hydroxy-3-methoxyphenyl)dodecane-3,5-dion

Inchi: InChI=1S/C19H28O4/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: QDSRAFNZQKMHPZ-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCCCCCCC(=O)CC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 320.42
CAS: 77334-06-6

Physical Properties

Property code	Value	Unit	Source
gf	-305.58	kJ/mol	Joback Method
hf	-745.12	kJ/mol	Joback Method
hfus	48.79	kJ/mol	Joback Method
hvap	89.74	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.222		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2560.10		NIST Webbook
rinpol	2560.10		NIST Webbook
tb	876.56	K	Joback Method
tc	1086.43	K	Joback Method
tf	576.64	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.98	J/mol×K	876.56	Joback Method
cpg	915.31	J/mol×K	1051.45	Joback Method
cpg	902.96	J/mol×K	1016.47	Joback Method
cpg	890.03	J/mol×K	981.49	Joback Method
cpg	876.43	J/mol×K	946.52	Joback Method
cpg	862.11	J/mol×K	911.54	Joback Method
cpg	927.13	J/mol×K	1086.43	Joback Method

dvisc	0.0000038	Pa×s	876.56	Joback Method
dvisc	0.0000054	Pa×s	826.57	Joback Method
dvisc	0.0000081	Pa×s	776.59	Joback Method
dvisc	0.0000128	Pa×s	726.60	Joback Method
dvisc	0.0000218	Pa×s	676.61	Joback Method
dvisc	0.0000403	Pa×s	626.63	Joback Method
dvisc	0.0000829	Pa×s	576.64	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77334066&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