3-(Hexadecyloxy)-2-benzofuran-1(3h)-one

Inchi: InChI=1S/C24H38O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-26-24-22-19-16-15-18-21
InchiKey: OZWCPSZFQNJWGZ-UHFFFAOYSA-N
Formula: C24H38O3
SMILES: CCCCCCCCCCCCCCCCCOC1OC(=O)c2ccccc21
Mol. weight [g/mol]: 374.56
CAS: 103034-71-5

Physical Properties

Property code	Value	Unit	Source
gf	1.02	kJ/mol	Joback Method
hf	-642.75	kJ/mol	Joback Method
hfus	58.38	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.353		Crippen Method
mcvol	327.710	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
tb	904.11	K	Joback Method
tc	1111.20	K	Joback Method
tf	534.14	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.85	J/mol×K	904.11	Joback Method
cpg	1122.62	J/mol×K	938.62	Joback Method
cpg	1140.09	J/mol×K	973.14	Joback Method
cpg	1156.33	J/mol×K	1007.65	Joback Method
cpg	1171.38	J/mol×K	1042.17	Joback Method
cpg	1185.29	J/mol×K	1076.68	Joback Method
cpg	1198.11	J/mol×K	1111.20	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=C103034715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume