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

Inchi: InChI=1S/C24H39NO2/c1-3-5-7-9-11-15-19-25(20-16-12-10-8-6-4-2)23-21-17-13-14-18-
InchiKey: WYPQQWBTOKVAQN-UHFFFAOYSA-N
Formula: C24H39NO2
SMILES: CCCCCCCCN(CCCCCCCC)C1OC(=O)c2ccccc21
Mol. weight [g/mol]: 373.57
CAS: 95817-71-3

Physical Properties

Property code	Value	Unit	Source
gf	216.80	kJ/mol	Joback Method
hf	-443.00	kJ/mol	Joback Method
hfus	60.21	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.879		Crippen Method
mcvol	331.820	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
tb	894.13	K	Joback Method
tc	1099.68	K	Joback Method
tf	544.38	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.44	J/mol×K	894.13	Joback Method
cpg	1135.77	J/mol×K	928.39	Joback Method
cpg	1153.89	J/mol×K	962.65	Joback Method
cpg	1170.88	J/mol×K	996.90	Joback Method
cpg	1186.81	J/mol×K	1031.16	Joback Method
cpg	1201.73	J/mol×K	1065.42	Joback Method
cpg	1215.74	J/mol×K	1099.68	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=C95817713&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