

2,5-Dibutyroxy-4-hydroxy butyrophenone

Inchi: InChI=1S/C18H24O6/c1-4-7-13(19)12-10-16(24-18(22)9-6-3)14(20)11-15(12)23-17(21)8
InchiKey: BBDHBFHJJJPZPV-UHFFFAOYSA-N
Formula: C18H24O6
SMILES: CCCC(=O)Oc1cc(C(=O)CCC)c(OC(=O)CCC)cc1O
Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-557.55	kJ/mol	Joback Method
hf	-980.75	kJ/mol	Joback Method
hfus	48.59	kJ/mol	Joback Method
hvap	97.33	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.786		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
tb	934.95	K	Joback Method
tc	1154.05	K	Joback Method
tf	650.05	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.43	J/mol×K	934.95	Joback Method
cpg	883.96	J/mol×K	1117.53	Joback Method
cpg	874.16	J/mol×K	1081.02	Joback Method
cpg	863.66	J/mol×K	1044.50	Joback Method
cpg	852.40	J/mol×K	1007.98	Joback Method
cpg	840.34	J/mol×K	971.47	Joback Method
cpg	893.11	J/mol×K	1154.05	Joback Method
dvisc	0.0000027	Pa×s	934.95	Joback Method
dvisc	0.0000037	Pa×s	887.47	Joback Method
dvisc	0.0000052	Pa×s	839.98	Joback Method

dvisc	0.0000077	Pa×s	792.50	Joback Method
dvisc	0.0000119	Pa×s	745.02	Joback Method
dvisc	0.0000196	Pa×s	697.53	Joback Method
dvisc	0.0000346	Pa×s	650.05	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000951&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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