

Benzophenone, 2,4,4'-trihydroxy-4'-laurate

Inchi:	InChI=1S/C25H32O5/c1-2-3-4-5-6-7-8-9-10-11-24(28)30-21-15-12-19(13-16-21)25(29)22
InchiKey:	CJJFPDOHTAEZLM-UHFFFAOYSA-N
Formula:	C25H32O5
SMILES:	CCCCCCCCCCCC(=O)Oc1ccc(C(=O)c2ccc(O)cc2O)cc1
Mol. weight [g/mol]:	412.52
CAS:	116495-93-3

Physical Properties

Property code	Value	Unit	Source
gf	-297.27	kJ/mol	Joback Method
hf	-809.74	kJ/mol	Joback Method
hfus	64.15	kJ/mol	Joback Method
hvap	118.39	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.155		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
tb	1121.14	K	Joback Method
tc	1372.75	K	Joback Method
tf	782.40	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.44	J/molxK	1121.14	Joback Method
cpg	1185.60	J/molxK	1163.07	Joback Method
cpg	1205.01	J/molxK	1205.01	Joback Method
cpg	1224.88	J/molxK	1246.94	Joback Method
cpg	1245.44	J/molxK	1288.88	Joback Method
cpg	1266.91	J/molxK	1330.81	Joback Method
cpg	1289.52	J/molxK	1372.75	Joback Method
dvisc	0.0000006	Paxs	782.40	Joback Method
dvisc	0.0000003	Paxs	838.86	Joback Method

dvisc	0.0000002	Paxs	895.31	Joback Method
dvisc	9.0760607e-08	Paxs	951.77	Joback Method
dvisc	5.5630259e-08	Paxs	1008.23	Joback Method
dvisc	3.5914538e-08	Paxs	1064.68	Joback Method
dvisc	2.4230873e-08	Paxs	1121.14	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=C116495933&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
mccvol:	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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