4-(n-Decyloxy)benzoic acid,4-(n-hexyloxy)phenyl ether

Other names: 4-n-Hexoxyphenyl-4'-n-decyloxybenzoate
Inchi: InChI=1S/C29H42O4/c1-3-5-7-9-10-11-12-14-24-31-26-17-15-25(16-18-26)29(30)33-28-
InchiKey: JBMARNOUPBCWIL-UHFFFAOYSA-N
Formula: C29H43O4
SMILES: CCCCCCCCCCOc1ccc(C(=O)Oc2ccc(OCCCCCC)cc2)cc1
Mol. weight [g/mol]: 455.65
CAS: 68162-09-4

Physical Properties

Property code	Value	Unit	Source
gf	-45.06	kJ/mol	Joback Method
hf	-701.01	kJ/mol	Joback Method
hfus	63.33	kJ/mol	Joback Method
hvap	100.00	kJ/mol	Joback Method
log10ws	-9.66		Crippen Method
logp	8.384		Crippen Method
mcvol	391.130	ml/mol	McGowan Method
pc	886.83	kPa	Joback Method
tb	1047.37	K	Joback Method
tc	1283.00	K	Joback Method
tf	611.09	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1407.09	J/mol×K	1283.00	Joback Method
cpg	1338.57	J/mol×K	1047.37	Joback Method
cpg	1354.45	J/mol×K	1086.64	Joback Method
cpg	1368.46	J/mol×K	1125.91	Joback Method
cpg	1380.68	J/mol×K	1165.19	Joback Method
cpg	1391.15	J/mol×K	1204.46	Joback Method
cpg	1399.93	J/mol×K	1243.73	Joback Method
dvisc	0.0000120	Pa×s	1047.37	Joback Method

dvisc	0.0001417	Pa×s	611.09	Joback Method
dvisc	0.0000755	Pa×s	683.80	Joback Method
dvisc	0.0000454	Pa×s	756.52	Joback Method
dvisc	0.0000298	Pa×s	829.23	Joback Method
dvisc	0.0000210	Pa×s	901.94	Joback Method
dvisc	0.0000156	Pa×s	974.66	Joback Method
hfust	31.70	kJ/mol	334.85	NIST Webbook

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=C68162094&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
hfust:	Enthalpy of fusion at a given temperature
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