4-Hexadecyloxybenzoic acid

Other names: p-Hexadecyloxybenzoic acid
Benzoic acid, 4-(hexadecyloxy)-
Inchi: InChI=1S/C23H38O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-26-22-18-16-21(17-19-22
InchiKey: GAQCVRTXIAGNEM-UHFFFAOYSA-N
Formula: C23H38O3
SMILES: CCCCCCCCCCCCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 362.55
CAS: 15872-48-7

Physical Properties

Property code	Value	Unit	Source
gf	-125.18	kJ/mol	Joback Method
hf	-690.02	kJ/mol	Joback Method
hfus	55.85	kJ/mol	Joback Method
hvap	95.56	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.245		Crippen Method
mcvol	324.480	ml/mol	McGowan Method
pc	1132.15	kPa	Joback Method
tb	925.77	K	Joback Method
tc	1133.44	K	Joback Method
tf	375.00 ± 1.00	K	NIST Webbook
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.54	J/mol×K	925.77	Joback Method
cpg	1092.53	J/mol×K	960.38	Joback Method
cpg	1108.35	J/mol×K	994.99	Joback Method
cpg	1123.05	J/mol×K	1029.61	Joback Method
cpg	1136.67	J/mol×K	1064.22	Joback Method
cpg	1149.28	J/mol×K	1098.83	Joback Method
cpg	1160.93	J/mol×K	1133.44	Joback Method

dvisc	0.0003152	Pa×s	520.89	Joback Method
dvisc	0.0001159	Pa×s	588.37	Joback Method
dvisc	0.0000523	Pa×s	655.85	Joback Method
dvisc	0.0000274	Pa×s	723.33	Joback Method
dvisc	0.0000160	Pa×s	790.81	Joback Method
dvisc	0.0000102	Pa×s	858.29	Joback Method
dvisc	0.0000069	Pa×s	925.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15872487&Units=SI
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

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