p-Undecyloxybenzoic acid

Other names: Benzoic acid, 4-(undecyloxy)-
4-n-undecyloxybenzoic acid
Inchi: InChI=1S/C18H28O3/c1-2-3-4-5-6-7-8-9-10-15-21-17-13-11-16(12-14-17)18(19)20/h11-1
InchiKey: NEJZHJHZOUISSH-UHFFFAOYSA-N
Formula: C18H28O3
SMILES: CCCCCCCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 292.41
CAS: 15872-44-3

Physical Properties

Property code	Value	Unit	Source
gf	-167.28	kJ/mol	Joback Method
hf	-586.82	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	84.44	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.294		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
tb	811.37	K	Joback Method
tc	1003.09	K	Joback Method
tf	369.00 ± 1.00	K	NIST Webbook
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.80	J/mol×K	811.37	Joback Method
cpg	791.76	J/mol×K	843.32	Joback Method
cpg	805.81	J/mol×K	875.28	Joback Method
cpg	819.00	J/mol×K	907.23	Joback Method
cpg	831.33	J/mol×K	939.19	Joback Method
cpg	842.86	J/mol×K	971.14	Joback Method
cpg	853.60	J/mol×K	1003.09	Joback Method

dvisc	0.0007195	Pa×s	464.54	Joback Method
dvisc	0.0002725	Pa×s	522.34	Joback Method
dvisc	0.0001253	Pa×s	580.15	Joback Method
dvisc	0.0000663	Pa×s	637.95	Joback Method
dvisc	0.0000390	Pa×s	695.76	Joback Method
dvisc	0.0000249	Pa×s	753.56	Joback Method
dvisc	0.0000169	Pa×s	811.37	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=C15872443&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume