4-(Decyloxy)benzoic acid

Other names:	p-Decyloxybenzoic acid
	4-n-Decyloxybenzoic acid
	Benzoic acid, 4-(decyloxy)-
Inchi:	InChI=1S/C17H26O3/c1-2-3-4-5-6-7-8-9-14-20-16-12-10-15(11-13-16)17(18)19/h10-13H
InchiKey:	NZNICZRIRMGOFG-UHFFFAOYSA-N
Formula:	C17H26O3
SMILES:	CCCCCCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	278.39
CAS:	5519-23-3

Physical Properties

Property code	Value	Unit	Source
gf	-175.70	kJ/mol	Joback Method
hf	-566.18	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.904		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
tb	788.49	K	Joback Method
tc	979.32	K	Joback Method
tf	453.27	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.51	J/mol×K	788.49	Joback Method
cpg	734.09	J/mol×K	820.29	Joback Method
cpg	747.80	J/mol×K	852.10	Joback Method
cpg	760.68	J/mol×K	883.90	Joback Method
cpg	772.74	J/mol×K	915.71	Joback Method
cpg	784.03	J/mol×K	947.51	Joback Method

cpg	794.55	J/mol×K	979.32	Joback Method
dvisc	0.0008446	Pa×s	453.27	Joback Method
dvisc	0.0003221	Pa×s	509.14	Joback Method
dvisc	0.0001487	Pa×s	565.01	Joback Method
dvisc	0.0000789	Pa×s	620.88	Joback Method
dvisc	0.0000464	Pa×s	676.75	Joback Method
dvisc	0.0000297	Pa×s	732.62	Joback Method
dvisc	0.0000202	Pa×s	788.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5519233&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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