p-Propoxybenzoic acid

Other names:	4-n-Propoxybenzoic acid
	4-n-propyloxybenzoic acid
	4-propyloxybenzoic acid
	Benzoic acid, 4-propoxy-
	Benzoic acid, p-propoxy-
	Para -4- Propoxy Benzoic Acid
	benzoic acid, 4-propyloxy-
	p-Propyloxybenzoic acid
	p-n-Propoxybenzoic acid
Inchi:	InChI=1S/C10H12O3/c1-2-7-13-9-5-3-8(4-6-9)10(11)12/h3-6H,2,7H2,1H3,(H,11,12)
InchiKey:	GDFUWFOCYZZGQU-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	180.20

Physical Properties

Property code	Value	Unit	Source
af	0.7840		Cheméo Relay (1.0)
hf	-503.15	kJ/mol	Cheméo Relay (1.0)
hfus	27.19	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hvap	93.71	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-2.94		Cheméo Relay (1.0)
logp	2.174		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	574.95	K	Cheméo Relay (1.0)
tc	772.22	K	Cheméo Relay (1.0)
tf	437.19	K	Cheméo Relay (1.0)
vc	0.512	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.22	J/mol×K	628.33	Joback Method
cpg	406.96	J/mol×K	827.77	Joback Method
cpg	398.96	J/mol×K	794.53	Joback Method
cpg	390.39	J/mol×K	761.29	Joback Method
cpg	381.24	J/mol×K	728.05	Joback Method
cpg	371.50	J/mol×K	694.81	Joback Method
cpg	361.17	J/mol×K	661.57	Joback Method
dvisc	0.0000978	Pa×s	586.00	Joback Method
dvisc	0.0000667	Pa×s	628.33	Joback Method
dvisc	0.0024094	Pa×s	374.38	Joback Method
dvisc	0.0001520	Pa×s	543.68	Joback Method
dvisc	0.0002546	Pa×s	501.35	Joback Method
dvisc	0.0004691	Pa×s	459.03	Joback Method
dvisc	0.0009783	Pa×s	416.70	Joback Method
hfust	16.74	kJ/mol	419.70	NIST Webbook
hfust	2.51	kJ/mol	426.70	NIST Webbook
hfust	7.95	kJ/mol	394.20	NIST Webbook
sfust	20.17	J/mol×K	394.20	NIST Webbook
sfust	39.89	J/mol×K	419.70	NIST Webbook
sfust	5.88	J/mol×K	426.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Thermodynamic Study of 4-n-Alkyloxybenzoic Acids: https://www.doi.org/10.1021/je900776y

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5438197&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume