Benzoic acid, 4-pentyl-

Other names:	4-Amylbenzoic acid
	4-Pentylbenzoic acid
	4-n-Pentylbenzoic acid
	Benzoic acid, p-pentyl-
	NSC 169024
	p-Amylbenzoic acid
	p-Pentylbenzoic acid
	p-n-Amylbenzoic acid
	p-n-Pentylbenzoic acid
	para-Pentylbenzoic acid
Inchi:	InChI=1S/C12H16O2/c1-2-3-4-5-10-6-8-11(9-7-10)12(13)14/h6-9H,2-5H2,1H3,(H,13,14)
InchiKey:	CWYNKKGQJYAHQG-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCCCc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	192.25
CAS:	26311-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-112.80	kJ/mol	Joback Method
hf	-330.76	kJ/mol	Joback Method
hfus	1.10	kJ/mol	Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids
hsub	118.20 ± 1.00	kJ/mol	NIST Webbook
hvap	68.67	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.117		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	651.67	K	Joback Method
tc	847.74	K	Joback Method
tf	374.69	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.06	J/mol×K	651.67	Joback Method
cpg	448.28	J/mol×K	717.03	Joback Method
cpg	488.76	J/mol×K	847.74	Joback Method
cpg	459.35	J/mol×K	749.71	Joback Method
cpg	469.77	J/mol×K	782.38	Joback Method
cpg	479.56	J/mol×K	815.06	Joback Method
cpg	436.53	J/mol×K	684.35	Joback Method
dvisc	0.0000958	Pa×s	605.51	Joback Method
dvisc	0.0001520	Pa×s	559.34	Joback Method
dvisc	0.0002621	Pa×s	513.18	Joback Method
dvisc	0.0005035	Pa×s	467.02	Joback Method
dvisc	0.0011159	Pa×s	420.85	Joback Method
dvisc	0.0000644	Pa×s	651.67	Joback Method
dvisc	0.0030088	Pa×s	374.69	Joback Method
hfust	1.50	kJ/mol	395.00	NIST Webbook
hfust	9.90	kJ/mol	362.00	NIST Webbook
hfust	2.60	kJ/mol	252.00	NIST Webbook
sfust	3.80	J/mol×K	395.00	NIST Webbook
sfust	27.35	J/mol×K	362.00	NIST Webbook
sfust	10.32	J/mol×K	252.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.26782e+01
Coeff. B	-4.02101e+03
Coeff. C	-8.95600e+01
Temperature range (K), min.	414.08
Temperature range (K), max.	635.39

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26311455&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids:	https://www.doi.org/10.1016/j.jct.2004.02.001
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
pvap:	Vapor 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