n-Propyl benzoate

Other names:	Benzoate de propyle
	Benzoic acid n-propyl ester
	Benzoic acid, propyl ester
	Propyl benzenecarboxylate
	Propyl benzoate
Inchi:	InChI=1S/C10H12O2/c1-2-8-12-10(11)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	UDEWPOVQBGFNGE-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	2315-68-6

Physical Properties

Property code	Value	Unit	Source
gf	-88.19	kJ/mol	Joback Method
hf	-258.00	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
log10ws	-2.67		Aqueous Solubility Prediction Method
logp	2.253		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	2600.00	kPa	Critical Point Measurements for n-Alkyl Benzoates (C8 to C13)
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1237.20		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1287.24		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1264.00		NIST Webbook

rinpol	1272.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1237.20		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1266.05		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1791.00		NIST Webbook
tb	503.00	K	NIST Webbook
tb	503.00	K	NIST Webbook
tb	504.00 ± 0.30	K	NIST Webbook
tb	504.00 ± 0.50	K	NIST Webbook
tb	504.10 ± 0.50	K	NIST Webbook
tb	503.90 ± 1.00	K	NIST Webbook
tc	743.85	K	Joback Method
tf	221.55	K	Aqueous Solubility Prediction Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	300.47	J/mol×K	531.17	Joback Method
cpg	314.07	J/mol×K	566.62	Joback Method
cpg	326.90	J/mol×K	602.06	Joback Method
cpg	338.99	J/mol×K	637.51	Joback Method
cpg	350.35	J/mol×K	672.95	Joback Method
cpg	361.01	J/mol×K	708.40	Joback Method
cpg	370.98	J/mol×K	743.85	Joback Method
dvisc	0.0012567	Pa×s	339.39	Joback Method
dvisc	0.0023380	Pa×s	301.04	Joback Method
dvisc	0.0007662	Pa×s	377.75	Joback Method
dvisc	0.0005118	Pa×s	416.11	Joback Method
dvisc	0.0003660	Pa×s	454.46	Joback Method
dvisc	0.0002757	Pa×s	492.81	Joback Method
dvisc	0.0002164	Pa×s	531.17	Joback Method
hvapt	60.20	kJ/mol	408.50	NIST Webbook
hvapt	52.70	kJ/mol	408.50	NIST Webbook
hvapt	53.80	kJ/mol	415.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	502.70	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54795e+01
Coeff. B	-5.04184e+03
Coeff. C	-3.99400e+01
Temperature range (K), min.	371.82
Temperature range (K), max.	535.80

Sources

Critical Point Measurements for n-Alkyl Benzoates (C8 to C13):	https://www.doi.org/10.1021/je700049s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2315686&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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume