Benzoic acid, phenyl ester

Other names: Phenyl benzoate
benzoin
Inchi: InChI=1S/C13H10O2/c14-13(11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1-10H
InchiKey: FCJSHPDYVMKCHI-UHFFFAOYSA-N
Formula: C13H10O2
SMILES: O=C(Oc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 198.22
CAS: 93-99-2

Physical Properties

Property code	Value	Unit	Source
chs	-6309.00 ± 15.00	kJ/mol	NIST Webbook
chs	-6304.00 ± 3.00	kJ/mol	NIST Webbook
gf	49.48	kJ/mol	Joback Method
hf	-150.00	kJ/mol	NIST Webbook
hf	-142.00 ± 3.00	kJ/mol	NIST Webbook
hf	-152.00 ± 4.70	kJ/mol	NIST Webbook
hfs	-241.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-238.00 ± 15.00	kJ/mol	NIST Webbook
hfs	-241.00 ± 2.00	kJ/mol	NIST Webbook
hfus	20.30	kJ/mol	Joback Method
hsub	99.00 ± 0.40	kJ/mol	NIST Webbook
hsub	99.00 ± 0.40	kJ/mol	NIST Webbook
hvap	58.24	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
ie	8.98 ± 0.05	eV	NIST Webbook
ie	8.80 ± 0.15	eV	NIST Webbook
ie	8.63	eV	NIST Webbook
ie	8.76	eV	NIST Webbook
log10ws	-2.85		Aqueous Solubility Prediction Method
logp	2.906		Crippen Method
mcvol	153.950	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	1604.00		NIST Webbook
ripol	2514.00		NIST Webbook
ripol	2514.00		NIST Webbook

tb	571.70	K	NIST Webbook
tc	874.68	K	Joback Method
tf	341.00 ± 3.00	K	NIST Webbook
tf	344.15 ± 1.50	K	NIST Webbook
tf	342.35	K	Aqueous Solubility Prediction Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.96	J/mol×K	874.68	Joback Method
cpg	366.53	J/mol×K	626.49	Joback Method
cpg	381.28	J/mol×K	667.85	Joback Method
cpg	394.82	J/mol×K	709.22	Joback Method
cpg	407.20	J/mol×K	750.58	Joback Method
cpg	418.48	J/mol×K	791.95	Joback Method
cpg	428.71	J/mol×K	833.31	Joback Method
dvisc	0.0001665	Pa×s	626.49	Joback Method
dvisc	0.0016739	Pa×s	361.27	Joback Method
dvisc	0.0009238	Pa×s	405.47	Joback Method
dvisc	0.0005731	Pa×s	449.68	Joback Method
dvisc	0.0003872	Pa×s	493.88	Joback Method
dvisc	0.0002790	Pa×s	538.08	Joback Method
dvisc	0.0002113	Pa×s	582.29	Joback Method
hvapt	62.40	kJ/mol	483.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52259e+01
Coeff. B	-5.68560e+03
Coeff. C	-5.10940e+01
Temperature range (K), min.	431.70
Temperature range (K), max.	624.56

Sources

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=C93992&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume