4-Butylbenzoic acid

Other names: Benzoic acid, 4-butyl-
p-n-Butylbenzoic acid
Inchi: InChI=1S/C11H14O2/c1-2-3-4-9-5-7-10(8-6-9)11(12)13/h5-8H,2-4H2,1H3,(H,12,13)
InchiKey: JFKUBRAOUZEZSL-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CCCCc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 178.23
CAS: 20651-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-121.22	kJ/mol	Joback Method
hf	-310.12	kJ/mol	Joback Method
hfus	0.76	kJ/mol	Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids
hsub	110.50 ± 0.70	kJ/mol	NIST Webbook
hvap	66.44	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.727		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	628.79	K	Joback Method
tc	827.28	K	Joback Method
tf	377.00 ± 1.00	K	NIST Webbook
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.63	J/mol×K	628.79	Joback Method
cpg	427.19	J/mol×K	794.20	Joback Method
cpg	417.93	J/mol×K	761.12	Joback Method
cpg	408.07	J/mol×K	728.04	Joback Method

cpg	397.58	J/mol×K	694.95	Joback Method
cpg	386.44	J/mol×K	661.87	Joback Method
cpg	435.88	J/mol×K	827.28	Joback Method
dvisc	0.0000758	Pa×s	628.79	Joback Method
dvisc	0.0001127	Pa×s	584.56	Joback Method
dvisc	0.0001788	Pa×s	540.33	Joback Method
dvisc	0.0003078	Pa×s	496.11	Joback Method
dvisc	0.0005896	Pa×s	451.88	Joback Method
dvisc	0.0013004	Pa×s	407.65	Joback Method
dvisc	0.0034768	Pa×s	363.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30427e+01
Coeff. B	-4.12031e+03
Coeff. C	-8.87680e+01
Temperature range (K), min.	411.80
Temperature range (K), max.	621.71

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20651712&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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume