4-Ethylbenzoic acid

Other names: Benzoic acid, 4-ethyl-
p-Ethylbenzoic acid
Inchi: InChI=1S/C9H10O2/c1-2-7-3-5-8(6-4-7)9(10)11/h3-6H,2H2,1H3,(H,10,11)
InchiKey: ZQVKTHRQIXSMGY-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: CCc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 150.17
CAS: 619-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-138.06	kJ/mol	Joback Method
hf	-355.60 ± 1.90	kJ/mol	NIST Webbook
hfs	-454.50 ± 1.90	kJ/mol	NIST Webbook
hfus	12.79	kJ/mol	Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids
hsub	98.90	kJ/mol	NIST Webbook
hsub	97.50 ± 2.50	kJ/mol	NIST Webbook
hsub	98.90 ± 0.20	kJ/mol	NIST Webbook
hsub	98.90 ± 0.20	kJ/mol	NIST Webbook
hsub	101.20 ± 0.80	kJ/mol	NIST Webbook
hvap	61.99	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.947		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	583.03	K	Joback Method
tc	787.21	K	Joback Method
tf	384.70 ± 0.00	K	NIST Webbook
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	325.89	J/mol×K	753.18	Joback Method
cpg	300.33	J/mol×K	651.09	Joback Method
cpg	290.68	J/mol×K	617.06	Joback Method
cpg	280.42	J/mol×K	583.03	Joback Method
cpg	309.40	J/mol×K	685.12	Joback Method
cpg	333.35	J/mol×K	787.21	Joback Method
cpg	317.91	J/mol×K	719.15	Joback Method
dvisc	0.0045711	Pa×s	340.88	Joback Method
dvisc	0.0001039	Pa×s	583.03	Joback Method
dvisc	0.0001544	Pa×s	542.67	Joback Method
dvisc	0.0002445	Pa×s	502.31	Joback Method
dvisc	0.0004197	Pa×s	461.95	Joback Method
dvisc	0.0007988	Pa×s	421.60	Joback Method
dvisc	0.0017423	Pa×s	381.24	Joback Method
hfust	14.06	kJ/mol	386.20	NIST Webbook
hfust	14.06	kJ/mol	386.20	NIST Webbook
hsubt	97.60 ± 0.20	kJ/mol	320.50	NIST Webbook
hsubt	98.20	kJ/mol	319.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46819e+01
Coeff. B	-4.60475e+03
Coeff. C	-8.71000e+01
Temperature range (K), min.	407.00
Temperature range (K), max.	578.51

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C619647&Units=SI

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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