3-Ethylbenzoic acid

Inchi: InChI=1S/C9H10O2/c1-2-7-4-3-5-8(6-7)9(10)11/h3-6H,2H2,1H3,(H,10,11)
InchiKey: HXUSUAKIRZZMGP-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: CCc1cccc(C(=O)O)c1
Mol. weight [g/mol]: 150.17
CAS: 619-20-5

Physical Properties

Property code	Value	Unit	Source
chs	-4524.90 ± 3.10	kJ/mol	NIST Webbook
gf	-138.06	kJ/mol	Joback Method
hf	-346.80 ± 1.50	kJ/mol	NIST Webbook
hfs	-445.90 ± 1.40	kJ/mol	NIST Webbook
hfus	18.41	kJ/mol	Joback Method
hsub	99.10 ± 2.50	kJ/mol	NIST Webbook
hsub	99.10	kJ/mol	NIST Webbook
hsub	99.10 ± 0.40	kJ/mol	NIST Webbook
hsub	99.70 ± 0.40	kJ/mol	NIST Webbook
hsub	99.70 ± 0.40	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	318.00 ± 4.00	K	NIST Webbook
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.42	J/mol×K	583.03	Joback Method
cpg	333.35	J/mol×K	787.21	Joback Method

cpg	325.89	J/mol×K	753.18	Joback Method
cpg	317.91	J/mol×K	719.15	Joback Method
cpg	309.40	J/mol×K	685.12	Joback Method
cpg	300.33	J/mol×K	651.09	Joback Method
cpg	290.68	J/mol×K	617.06	Joback Method
cps	199.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0017423	Pa×s	381.24	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	0.0045711	Pa×s	340.88	Joback Method
hsubt	99.10	kJ/mol	309.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C619205&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume