

2-Ethylbenzoic acid

Inchi:	InChI=1S/C9H10O2/c1-2-7-5-3-4-6-8(7)9(10)11/h3-6H,2H2,1H3,(H,10,11)
InchiKey:	CGMMPMYKMDITEA-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CCc1ccccc1C(=O)O
Mol. weight [g/mol]:	150.17
CAS:	612-19-1

Physical Properties

Property code	Value	Unit	Source
chs	-4529.40 ± 3.70	kJ/mol	NIST Webbook
gf	-138.06	kJ/mol	Joback Method
hf	-340.70 ± 1.50	kJ/mol	NIST Webbook
hfs	-441.40 ± 1.50	kJ/mol	NIST Webbook
hfus	18.41	kJ/mol	Joback Method
hsub	100.70	kJ/mol	NIST Webbook
hsub	101.10 ± 0.40	kJ/mol	NIST Webbook
hsub	101.10 ± 0.40	kJ/mol	NIST Webbook
hsub	100.70 ± 2.50	kJ/mol	NIST Webbook
hsub	100.70 ± 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	532.20	K	NIST Webbook
tc	787.21	K	Joback Method
tf	338.00 ± 3.00	K	NIST Webbook
vc	0.457	m ³ /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/molxK	753.18	Joback Method
cpg	317.91	J/molxK	719.15	Joback Method
cpg	309.40	J/molxK	685.12	Joback Method
cpg	300.33	J/molxK	651.09	Joback Method
cpg	290.68	J/molxK	617.06	Joback Method
cps	208.70	J/molxK	298.15	NIST Webbook
dvisc	0.0017423	Paxs	381.24	Joback Method
dvisc	0.0001039	Paxs	583.03	Joback Method
dvisc	0.0001544	Paxs	542.67	Joback Method
dvisc	0.0002445	Paxs	502.31	Joback Method
dvisc	0.0004197	Paxs	461.95	Joback Method
dvisc	0.0007988	Paxs	421.60	Joback Method
dvisc	0.0045711	Paxs	340.88	Joback Method
hsubt	100.50	kJ/mol	305.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C612191&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

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