

(2E)-2-ethyl-3-phenyl-2-propenoic acid

Inchi:	InChI=1S/C11H12O2/c1-2-10(11(12)13)8-9-6-4-3-5-7-9/h3-8H,2H2,1H3,(H,12,13)/b10-8
InchiKey:	RUETZBUVTWCCIZ-CSKARUKUSA-N
Formula:	C11H12O2
SMILES:	CCC(=Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	176.21

Physical Properties

Property code	Value	Unit	Source
gf	-39.92	kJ/mol	Joback Method
hf	-191.22	kJ/mol	Joback Method
hfus	22.87	kJ/mol	Joback Method
hvap	65.82	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.565		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	627.85	K	Joback Method
tc	836.58	K	Joback Method
tf	331.86	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.93	J/mol×K	627.85	Joback Method
cpg	365.47	J/mol×K	662.64	Joback Method
cpg	376.24	J/mol×K	697.43	Joback Method
cpg	386.30	J/mol×K	732.21	Joback Method
cpg	395.69	J/mol×K	767.00	Joback Method
cpg	404.47	J/mol×K	801.79	Joback Method
cpg	412.68	J/mol×K	836.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004865&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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