3-Phenylbutyric acid

Other names: «beta»-Phenyl-n-butyric acid
Benzenepropanoic acid, «beta»-methyl-
3-Phenylbutanoic acid
Inchi: InChI=1S/C10H12O2/c1-8(7-10(11)12)9-5-3-2-4-6-9/h2-6,8H,7H2,1H3,(H,11,12)
InchiKey: ZZEWMYILWXCRHZ-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(CC(=O)O)c1ccccc1
Mol. weight [g/mol]: 164.20
CAS: 4593-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-122.45	kJ/mol	Joback Method
hf	-283.29	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.265		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	600.49	K	Joback Method
tc	804.72	K	Joback Method
tf	324.63	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.11	J/mol×K	600.49	Joback Method
cpg	339.69	J/mol×K	634.53	Joback Method
cpg	350.55	J/mol×K	668.57	Joback Method
cpg	360.71	J/mol×K	702.61	Joback Method
cpg	370.22	J/mol×K	736.64	Joback Method
cpg	379.10	J/mol×K	770.68	Joback Method

cpg	387.38	J/mol×K	804.72	Joback Method
dvisc	0.0090484	Pa×s	324.63	Joback Method
dvisc	0.0025745	Pa×s	370.61	Joback Method
dvisc	0.0009668	Pa×s	416.58	Joback Method
dvisc	0.0004411	Pa×s	462.56	Joback Method
dvisc	0.0002319	Pa×s	508.54	Joback Method
dvisc	0.0001356	Pa×s	554.51	Joback Method
dvisc	0.0000861	Pa×s	600.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.20	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4593902&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume