Benzoylacrylic acid

Other names:	2-Butenoic acid, 4-oxo-4-phenyl-
	3-Benzoylacrylic acid
	Acrylic acid, 3-benzoyl-
	Crotonic acid, 4-oxo-4-phenyl-
	«beta»-Benzoylacrylic acid
	4-Oxo-4-phenyl-2-butenoic acid
	NSC 143
Inchi:	InChI=1S/C10H8O3/c11-9(6-7-10(12)13)8-4-2-1-3-5-8/h1-7H,(H,12,13)/b7-6+
InchiKey:	PLPDHGOODMBBGN-VOTSOKGWSA-N
Formula:	C10H8O3
SMILES:	O=C(O)C=CC(=O)c1ccccc1
Mol. weight [g/mol]:	176.17
CAS:	583-06-2

Physical Properties

Property code	Value	Unit	Source
gf	-168.71	kJ/mol	Joback Method
hf	-273.37	kJ/mol	Joback Method
hfus	23.18	kJ/mol	Joback Method
hvap	70.26	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.510		Crippen Method
mcvol	132.710	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	658.96	K	Joback Method
tc	874.35	K	Joback Method
tf	384.48	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.48	J/mol×K	658.96	Joback Method
cpg	326.80	J/mol×K	694.86	Joback Method

cpg	335.42	J/mol×K	730.76	Joback Method
cpg	343.40	J/mol×K	766.66	Joback Method
cpg	350.78	J/mol×K	802.56	Joback Method
cpg	357.61	J/mol×K	838.45	Joback Method
cpg	363.94	J/mol×K	874.35	Joback Method
dvisc	0.0029239	Pa×s	384.48	Joback Method
dvisc	0.0011188	Pa×s	430.23	Joback Method
dvisc	0.0005149	Pa×s	475.97	Joback Method
dvisc	0.0002715	Pa×s	521.72	Joback Method
dvisc	0.0001587	Pa×s	567.47	Joback Method
dvisc	0.0001006	Pa×s	613.21	Joback Method
dvisc	0.0000679	Pa×s	658.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C583062&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume