Benzenebutanal

Other names:	Butyraldehyde, 4-phenyl- «gamma»-Phenylbutyraldehyde 4-Phenylbutanal 4-Phenylbutyraldehyde
Inchi:	InChI=1S/C10H12O/c11-9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7,9H,4-5,8H2
InchiKey:	NHFRGTVSKOPUBK-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	O=CCCCc1ccccc1
Mol. weight [g/mol]:	148.20
CAS:	18328-11-5

Physical Properties

Property code	Value	Unit	Source
gf	46.21	kJ/mol	Joback Method
hf	-98.78	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	46.85	kJ/mol	Joback Method
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.208		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	503.54	K	Joback Method
tc	713.04	K	Joback Method
tf	270.88	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.72	J/mol×K	503.54	Joback Method
cpg	291.30	J/mol×K	538.46	Joback Method
cpg	304.07	J/mol×K	573.37	Joback Method
cpg	316.07	J/mol×K	608.29	Joback Method

cpg	327.32	J/mol×K	643.21	Joback Method
cpg	337.86	J/mol×K	678.13	Joback Method
cpg	347.73	J/mol×K	713.04	Joback Method
dvisc	0.0035007	Pa×s	270.88	Joback Method
dvisc	0.0017677	Pa×s	309.66	Joback Method
dvisc	0.0010392	Pa×s	348.43	Joback Method
dvisc	0.0006795	Pa×s	387.21	Joback Method
dvisc	0.0004801	Pa×s	425.99	Joback Method
dvisc	0.0003594	Pa×s	464.76	Joback Method
dvisc	0.0002813	Pa×s	503.54	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18328115&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
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
ie: Ionization energy
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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