BENZENEACETALDEHYDE, .ALPHA.-ETHYL-

Other names: 2-phenylbutyraldehyde
Inchi: InChI=1S/C10H12O/c1-2-9(8-11)10-6-4-3-5-7-10/h3-9H,2H2,1H3
InchiKey: DIBSCKQIZZVKMG-UHFFFAOYSA-N
Formula: C10H12O
SMILES: CCC(C=O)c1ccccc1
Mol. weight [g/mol]: 148.21

Physical Properties

Property code	Value	Unit	Source
af	0.3840		Cheméo Relay (1.0)
hf	-94.38	kJ/mol	Cheméo Relay (1.0)
hfus	14.46	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
logp	2.379		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	490.10	K	Cheméo Relay (1.0)
tc	714.49	K	Cheméo Relay (1.0)
tf	278.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.96	J/mol×K	503.10	Joback Method
cpg	291.94	J/mol×K	538.82	Joback Method
cpg	305.05	J/mol×K	574.54	Joback Method
cpg	317.35	J/mol×K	610.25	Joback Method
cpg	328.85	J/mol×K	645.97	Joback Method
cpg	339.61	J/mol×K	681.69	Joback Method
cpg	349.65	J/mol×K	717.41	Joback Method
dvisc	0.0048874	Pa×s	255.88	Joback Method
dvisc	0.0021490	Pa×s	297.08	Joback Method
dvisc	0.0011543	Pa×s	338.29	Joback Method

dvisc	0.0007096	Pa×s	379.49	Joback Method
dvisc	0.0004798	Pa×s	420.69	Joback Method
dvisc	0.0003479	Pa×s	461.90	Joback Method
dvisc	0.0002659	Pa×s	503.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2439432&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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