

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]:	148.20
CAS:	2439-43-2

Physical Properties

Property code	Value	Unit	Source
gf	43.77	kJ/mol	Joback Method
hf	-104.06	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	46.46	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.379		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	503.10	K	Joback Method
tc	717.41	K	Joback Method
tf	255.88	K	Joback Method
vc	0.498	m ³ /kmol	Joback Method

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	Paxs	255.88	Joback Method

dvisc	0.0021490	Paxs	297.08	Joback Method
dvisc	0.0011543	Paxs	338.29	Joback Method
dvisc	0.0007096	Paxs	379.49	Joback Method
dvisc	0.0004798	Paxs	420.69	Joback Method
dvisc	0.0003479	Paxs	461.90	Joback Method
dvisc	0.0002659	Paxs	503.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2439432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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