Benzeneacetaldehyde, «alpha»-(phenylmethylene)-

Inchi: InChI=1S/C15H12O/c16-12-15(14-9-5-2-6-10-14)11-13-7-3-1-4-8-13/h1-12H/b15-11+

InchiKey: JYVONCAJVKBEGI-RVDMUPIBSA-N

Formula: C15H12O

SMILES: O=CC(=Cc1ccccc1)c1ccccc1

Mol. weight [g/mol]: 208.26

CAS: 13702-35-7

Physical Properties

Property code	Value	Unit	Source
gf	272.39	kJ/mol	Joback Method
hf	141.98	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	60.29	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.426		Crippen Method
mcvol	171.960	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	648.66	K	Joback Method
tc	899.57	K	Joback Method
tf	334.61	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.36	J/mol×K	648.66	Joback Method
cpg	434.92	J/mol×K	690.48	Joback Method
cpg	449.14	J/mol×K	732.30	Joback Method
cpg	462.13	J/mol×K	774.11	Joback Method
cpg	474.01	J/mol×K	815.93	Joback Method
cpg	484.90	J/mol×K	857.75	Joback Method
cpg	494.91	J/mol×K	899.57	Joback Method

Sources

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=C13702357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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