Benzeneacetaldehyde, «alpha»-methyl-4-(1,1-dimethylethyl)

Inchi: InChI=1S/C13H18O/c1-10(9-14)11-5-7-12(8-6-11)13(2,3)4/h5-10H,1-4H3

InchiKey: SNOVXNPIRUDJNG-UHFFFAOYSA-N

Formula: C13H18O

SMILES: CC(C=O)c1ccc(C(C)(C)C)cc1

Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
hf	-192.14	kJ/mol	Cheméo Relay (1.0)
hfus	14.43	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Cheméo Relay (1.0)
ie	8.34	eV	Cheméo Relay (1.0)
logp	3.287		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1391.00		NIST Webbook
tb	522.67	K	Cheméo Relay (1.0)
tc	750.60	K	Cheméo Relay (1.0)
tf	324.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.75	J/mol×K	573.49	Joback Method
cpg	506.68	J/mol×K	791.49	Joback Method
cpg	494.76	J/mol×K	755.15	Joback Method
cpg	481.95	J/mol×K	718.82	Joback Method
cpg	468.21	J/mol×K	682.49	Joback Method
cpg	453.47	J/mol×K	646.16	Joback Method
cpg	437.67	J/mol×K	609.82	Joback Method
dvisc	0.0005501	Pa×s	439.06	Joback Method
dvisc	0.0001904	Pa×s	573.49	Joback Method
dvisc	0.0002554	Pa×s	528.68	Joback Method
dvisc	0.0003617	Pa×s	483.87	Joback Method

dvisc	0.0040558	Pa×s	304.63	Joback Method
dvisc	0.0009203	Pa×s	394.25	Joback Method
dvisc	0.0017567	Pa×s	349.44	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R635588&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point