

Benzene ethanal,4-[1,1-dimethyl]-, «alpha»-methyl-

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	1441.30		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	437.67	J/mol×K	609.82	Joback Method
cpg	453.47	J/mol×K	646.16	Joback Method
cpg	468.21	J/mol×K	682.49	Joback Method
cpg	481.95	J/mol×K	718.82	Joback Method
cpg	494.76	J/mol×K	755.15	Joback Method
cpg	506.68	J/mol×K	791.49	Joback Method
dvisc	0.0040558	Pa×s	304.63	Joback Method
dvisc	0.0017567	Pa×s	349.44	Joback Method
dvisc	0.0009203	Pa×s	394.25	Joback Method
dvisc	0.0005501	Pa×s	439.06	Joback Method

dvisc	0.0003617	Pa×s	483.87	Joback Method
dvisc	0.0002554	Pa×s	528.68	Joback Method
dvisc	0.0001904	Pa×s	573.49	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515598&Units=SI

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

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