CYCLAMEN ALDEHYDE

Other names:	«alpha»-Methyl-p-isopropylhydrocinnamic aldehyde 3-(p-Isopropylphenyl)isobutyraldehyde Benzenepropanal, «alpha»-methyl-4-(1-methylethyl)- Hydrocinnamaldehyde, p-isopropyl-«alpha»-methyl- Aldehyde B Cyclamal Cyclamen aldehyde p-Isopropyl-«alpha»-methylhydrocinnamaldehyde p-Isopropyl-«alpha»-methylhydrocinnamic aldehyde p-Isopropyl-«alpha»-methylphenylpropyl aldehyde «alpha»-Methyl-p-isopropylhydrocinnamaldehyde 2-Methyl-3-(p-isopropylphenyl)propionaldehyde «beta»-Methyl-p-iso-propyl phenyl propionaldehyde 2-Methyl-3-(4-isopropylphenyl)-propanal 3-(p-Isopropylphenyl)-2-methylpropionaldehyde 3-p-Cumenyl-2-methylpropionaldehyde Cymal
Inchi:	InChI=1S/C13H18O/c1-10(2)13-6-4-12(5-7-13)8-11(3)9-14/h4-7,9-11H,8H2,1-3H3
InchiKey:	ZFNVDHOSLNRHNN-UHFFFAOYSA-N
Formula:	C13H18O
SMILES:	CC(C=O)Cc1ccc(C(C)C)cc1
Mol. weight [g/mol]:	190.29

Physical Properties

Property code	Value	Unit	Source
hfus	18.32	kJ/mol	Joback Method
hvap	72.60	kJ/mol	NIST Webbook
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-3.49		Cheméo Relay (1.0)
logp	3.188		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1436.50		NIST Webbook
rinpol	1424.10		NIST Webbook
rinpol	1424.30		NIST Webbook
rinpol	1424.10		NIST Webbook
rinpol	1436.50		NIST Webbook

tb	529.44	K	Cheméo Relay (1.0)
tc	746.58	K	Cheméo Relay (1.0)
tf	276.81	K	Cheméo Relay (1.0)
vc	0.622	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.91	J/mol×K	576.28	Joback Method
cpg	434.26	J/mol×K	611.24	Joback Method
cpg	449.65	J/mol×K	646.19	Joback Method
cpg	464.14	J/mol×K	681.15	Joback Method
cpg	477.75	J/mol×K	716.10	Joback Method
cpg	490.51	J/mol×K	751.06	Joback Method
cpg	502.48	J/mol×K	786.01	Joback Method
dvisc	0.0044374	Pa×s	287.21	Joback Method
dvisc	0.0018172	Pa×s	335.39	Joback Method
dvisc	0.0009313	Pa×s	383.57	Joback Method
dvisc	0.0005541	Pa×s	431.75	Joback Method
dvisc	0.0003659	Pa×s	479.92	Joback Method
dvisc	0.0002606	Pa×s	528.10	Joback Method
dvisc	0.0001964	Pa×s	576.28	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=C103957&Units=SI

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

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
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
vc:	Critical Volume