

Cyclohexanecarboxylic acid

Other names:	Benzoic acid, hexahydro- Carboxycyclohexane Cyclohexylcarboxylic acid Cyclohexylmethanoic acid Hexahydrobenzoic acid
Inchi:	InChI=1S/C7H12O2/c8-7(9)6-4-2-1-3-5-6/h6H,1-5H2,(H,8,9)
InchiKey:	NZNMSOKMUBTKW-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	O=C(O)C1CCCCC1
Mol. weight [g/mol]:	128.17
CAS:	98-89-5

Physical Properties

Property code	Value	Unit	Source
affp	823.80	kJ/mol	NIST Webbook
basg	792.80	kJ/mol	NIST Webbook
chs	-3883.70 ± 0.30	kJ/mol	NIST Webbook
gf	-233.23	kJ/mol	Joback Method
hf	-398.30	kJ/mol	Joback Method
hfus	11.41	kJ/mol	Joback Method
hvap	55.03	kJ/mol	Joback Method
log10ws	-1.45		Aqueous Solubility Prediction Method
logp	1.651		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1127.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	505.70 ± 1.00	K	NIST Webbook
tb	505.70	K	NIST Webbook
tc	727.55	K	Joback Method
tf	304.00 ± 4.00	K	NIST Webbook
tf	298.50 ± 0.50	K	NIST Webbook

tf	302.00 ± 2.00	K	NIST Webbook
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.88	J/mol×K	558.89	Joback Method
cpg	275.06	J/mol×K	592.62	Joback Method
cpg	286.55	J/mol×K	626.36	Joback Method
cpg	297.37	J/mol×K	660.09	Joback Method
cpg	307.54	J/mol×K	693.82	Joback Method
cpg	249.99	J/mol×K	525.16	Joback Method
cpg	317.07	J/mol×K	727.55	Joback Method
dvisc	0.0132000	Paxs	310.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0092600	Paxs	320.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0067600	Paxs	330.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
dvisc	0.0050700	Paxs	340.00	Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material)
hfust	9.20	kJ/mol	301.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.70	K	1.70	NIST Webbook

Sources

Temperature and composition dependence of the density and viscosity of binary mixtures of (1-decanol + fragrance material):	https://www.doi.org/10.1016/j.tca.2009.02.013
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Solubility of fragrance raw materials in water: Experimental study, correlations, and Mod. UNIFAC (Do predictions:	https://www.doi.org/10.1016/j.jct.2010.07.013

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolt:	Non-polar retention indices
ripolt:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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