1,4-BENZODIOXAN-6-CARBOXALDEHYDE

Other names: 1,4-Benzodioxin-6-carboxaldehyde, 2,3-dihydro-
7-Formyl-1,4-benzodioxane
2,3-dihydro-1,4-benzodioxin-6-carbaldehyde
Inchi: InChI=1S/C9H8O3/c10-6-7-1-2-8-9(5-7)12-4-3-11-8/h1-2,5-6H,3-4H2
InchiKey: CWKXDPPQCVWXAG-UHFFFAOYSA-N
Formula: C9H8O3
SMILES: O=Cc1ccc2c(c1)OCCO2
Mol. weight [g/mol]: 164.16

Physical Properties

Property code	Value	Unit	Source
hfus	25.54	kJ/mol	Joback Method
hsub	98.20 ± 1.40	kJ/mol	NIST Webbook
hvap	74.20	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-2.28		Cheméo Relay (1.0)
logp	1.270		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
tb	557.42	K	Cheméo Relay (1.0)
tf	358.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.30	J/mol×K	757.52	Joback Method
cpg	331.28	J/mol×K	796.98	Joback Method
cpg	284.06	J/mol×K	599.66	Joback Method
cpg	295.08	J/mol×K	639.13	Joback Method
cpg	305.25	J/mol×K	678.59	Joback Method
cpg	314.64	J/mol×K	718.06	Joback Method
cpg	272.15	J/mol×K	560.20	Joback Method
dvisc	0.0011988	Pa×s	424.37	Joback Method
dvisc	0.0016917	Pa×s	390.41	Joback Method
dvisc	0.0025492	Pa×s	356.45	Joback Method

dvisc	0.0008940	Pa×s	458.33	Joback Method
dvisc	0.0006942	Pa×s	492.28	Joback Method
dvisc	0.0005570	Pa×s	526.24	Joback Method
dvisc	0.0004590	Pa×s	560.20	Joback Method
hfust	19.44	kJ/mol	324.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	2.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29668448&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
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation 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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point