1,4-Benzodioxin

Inchi: InChI=1S/C8H6O2/c1-2-4-8-7(3-1)9-5-6-10-8/h1-6H
InchiKey: HPARLNRMYDSBNO-UHFFFAOYSA-N
Formula: C8H6O2
SMILES: C1=COc2ccccc2O1
Mol. weight [g/mol]: 134.13
CAS: 255-37-8

Physical Properties

Property code	Value	Unit	Source
gf	33.34	kJ/mol	Joback Method
hf	-102.63	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	46.05	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.929		Crippen Method
mcvol	96.400	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	466.00	K	NIST Webbook
tc	722.27	K	Joback Method
tf	291.42	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.66	J/mol×K	482.84	Joback Method
cpg	209.32	J/mol×K	522.74	Joback Method
cpg	220.02	J/mol×K	562.65	Joback Method
cpg	229.83	J/mol×K	602.55	Joback Method
cpg	238.82	J/mol×K	642.46	Joback Method
cpg	247.05	J/mol×K	682.36	Joback Method
cpg	254.58	J/mol×K	722.27	Joback Method
dvisc	0.0025598	Pa×s	291.42	Joback Method
dvisc	0.0016212	Pa×s	323.32	Joback Method

dvisc	0.0011145	Pa×s	355.23	Joback Method
dvisc	0.0008150	Pa×s	387.13	Joback Method
dvisc	0.0006251	Pa×s	419.03	Joback Method
dvisc	0.0004977	Pa×s	450.94	Joback Method
dvisc	0.0004085	Pa×s	482.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.00 ± 1.00	K	2.10	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C255378&Units=SI
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
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume