4H-1,3-Benzodioxin

Other names: 1,3-Benzodioxan
Inchi: InChI=1S/C8H8O2/c1-2-4-8-7(3-1)5-9-6-10-8/h1-4H,5-6H2
InchiKey: TWSIYGATPWEKBK-UHFFFAOYSA-N
Formula: C8H8O2
SMILES: c1ccc2c(c1)COCO2
Mol. weight [g/mol]: 136.15
CAS: 254-27-3

Physical Properties

Property code	Value	Unit	Source
gf	3.38	kJ/mol	Joback Method
hf	-160.41	kJ/mol	Joback Method
hfus	21.05	kJ/mol	Joback Method
hvap	45.75	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.553		Crippen Method
mcvol	100.700	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
tb	483.68	K	Joback Method
tc	720.55	K	Joback Method
tf	285.60	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.77	J/mol×K	483.68	Joback Method
cpg	226.87	J/mol×K	523.16	Joback Method
cpg	238.97	J/mol×K	562.64	Joback Method
cpg	250.14	J/mol×K	602.12	Joback Method
cpg	260.44	J/mol×K	641.59	Joback Method
cpg	269.93	J/mol×K	681.07	Joback Method
cpg	278.67	J/mol×K	720.55	Joback Method
dvisc	0.0030174	Pa×s	290.66	Joback Method

dvisc	0.0018387	Pa×s	322.83	Joback Method
dvisc	0.0012257	Pa×s	355.00	Joback Method
dvisc	0.0008740	Pa×s	387.17	Joback Method
dvisc	0.0006564	Pa×s	419.34	Joback Method
dvisc	0.0005135	Pa×s	451.51	Joback Method
dvisc	0.0004151	Pa×s	483.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	483.50 ± 0.50	K	101.00	NIST Webbook
tbrp	374.10 ± 0.50	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C254273&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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