2H-1,5-Benzodioxepin, 3,4-dihydro-

Other names: Pyrocatechol trimethylene ether
Inchi: InChI=1S/C9H10O2/c1-2-5-9-8(4-1)10-6-3-7-11-9/h1-2,4-5H,3,6-7H2
InchiKey: CBXMULHQEVXJDI-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: c1ccc2c(c1)OCCCO2
Mol. weight [g/mol]: 150.17
CAS: 7216-18-4

Physical Properties

Property code	Value	Unit	Source
chl	-4729.59 ± 0.84	kJ/mol	NIST Webbook
gf	-0.30	kJ/mol	Joback Method
hf	-187.21	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	55.56	kJ/mol	NIST Webbook
log10ws	-2.02		Crippen Method
logp	1.848		Crippen Method
mcvol	114.790	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	510.83	K	Joback Method
tc	752.56	K	Joback Method
tf	298.41	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.99	J/mol×K	510.83	Joback Method
cpg	321.13	J/mol×K	712.27	Joback Method
cpg	310.09	J/mol×K	671.98	Joback Method
cpg	298.12	J/mol×K	631.69	Joback Method
cpg	285.15	J/mol×K	591.41	Joback Method
cpg	271.13	J/mol×K	551.12	Joback Method
cpg	331.28	J/mol×K	752.56	Joback Method

dvisc	0.0003211	Pa×s	510.83	Joback Method
dvisc	0.0004146	Pa×s	475.43	Joback Method
dvisc	0.0005577	Pa×s	440.02	Joback Method
dvisc	0.0007902	Pa×s	404.62	Joback Method
dvisc	0.0011969	Pa×s	369.22	Joback Method
dvisc	0.0019800	Pa×s	333.81	Joback Method
dvisc	0.0036911	Pa×s	298.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7216184&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid 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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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