1,3-Dioxepane

Inchi: InChI=1S/C5H10O2/c1-2-4-7-5-6-3-1/h1-5H2
InchiKey: CZLMRJZAHXYRIX-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: C1CCOCOC1
Mol. weight [g/mol]: 102.13
CAS: 505-65-7

Physical Properties

Property code	Value	Unit	Source
chl	-3009.00	kJ/mol	NIST Webbook
gf	-160.96	kJ/mol	Joback Method
hf	-342.03	kJ/mol	Joback Method
hfus	13.33	kJ/mol	Joback Method
hvap	36.65	kJ/mol	Joback Method
ie	9.45	eV	NIST Webbook
log10ws	-0.48		Crippen Method
logp	0.771		Crippen Method
mcvol	82.190	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
rinpol	802.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	795.00		NIST Webbook
ripol	1176.00		NIST Webbook
sg	338.60 ± 4.80	J/mol×K	NIST Webbook
tb	396.19	K	Joback Method
tc	612.99	K	Joback Method
tf	207.35	K	Joback Method
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.40	J/mol×K	396.19	Joback Method

cpg	223.65	J/mol×K	612.99	Joback Method
cpg	213.40	J/mol×K	576.86	Joback Method
cpg	202.51	J/mol×K	540.73	Joback Method
cpg	190.98	J/mol×K	504.59	Joback Method
cpg	178.79	J/mol×K	468.46	Joback Method
cpg	165.94	J/mol×K	432.32	Joback Method
cpl	167.00	J/mol×K	298.00	NIST Webbook
dvisc	0.0078305	Pa×s	238.82	Joback Method
dvisc	0.0003793	Pa×s	396.19	Joback Method
dvisc	0.0005639	Pa×s	364.72	Joback Method
dvisc	0.0009034	Pa×s	333.24	Joback Method
dvisc	0.0015970	Pa×s	301.77	Joback Method
dvisc	0.0032237	Pa×s	270.30	Joback Method
dvisc	0.0249022	Pa×s	207.35	Joback Method
hvapt	41.00	kJ/mol	293.00	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=C505657&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase 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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume