1,3,5-Trioxepane

Other names: 1,3,5-Trioxacycloheptane
Inchi: InChI=1S/C4H8O3/c1-2-6-4-7-3-5-1/h1-4H2
InchiKey: ULAGGPJVDRGWTI-UHFFFAOYSA-N
Formula: C4H8O3
SMILES: C1COCOCO1
Mol. weight [g/mol]: 104.10
CAS: 5981-06-6

Physical Properties

Property code	Value	Unit	Source
gf	-255.50	kJ/mol	Joback Method
hf	-453.39	kJ/mol	Joback Method
hfus	18.72	kJ/mol	Joback Method
hvap	38.94	kJ/mol	Joback Method
ie	9.62	eV	NIST Webbook
log10ws	0.36		Crippen Method
logp	-0.035		Crippen Method
mcvol	73.970	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
rinpol	771.00		NIST Webbook
rinpol	793.00		NIST Webbook
tb	400.26	K	Joback Method
tc	619.45	K	Joback Method
tf	222.65	K	Joback Method
vc	0.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.58	J/mol×K	400.26	Joback Method
cpg	195.39	J/mol×K	582.92	Joback Method
cpg	185.98	J/mol×K	546.39	Joback Method
cpg	175.99	J/mol×K	509.85	Joback Method
cpg	165.43	J/mol×K	473.32	Joback Method

cpg	154.30	J/mol×K	436.79	Joback Method
cpg	204.25	J/mol×K	619.45	Joback Method
dvisc	0.0004402	Pa×s	400.26	Joback Method
dvisc	0.0006500	Pa×s	370.66	Joback Method
dvisc	0.0010269	Pa×s	341.06	Joback Method
dvisc	0.0017697	Pa×s	311.45	Joback Method
dvisc	0.0034190	Pa×s	281.85	Joback Method
dvisc	0.0077099	Pa×s	252.25	Joback Method
dvisc	0.0215820	Pa×s	222.65	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5981066&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

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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