2,4,7-Trioxepane, 6-methyl

Inchi: InChI=1S/C5H10O3/c1-5-2-6-3-7-4-8-5/h5H,2-4H2,1H3
InchiKey: UZLVVHHXLVCCDM-UHFFFAOYSA-N
Formula: C5H10O3
SMILES: CC1COCOCO1
Mol. weight [g/mol]: 118.13

Physical Properties

Property code	Value	Unit	Source
gf	-254.79	kJ/mol	Joback Method
hf	-494.37	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	40.86	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	0.353		Crippen Method
mcvol	88.060	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
rinpol	812.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	812.00		NIST Webbook
tb	418.47	K	Joback Method
tc	634.66	K	Joback Method
tf	229.68	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.18	J/mol×K	418.47	Joback Method
cpg	194.62	J/mol×K	454.50	Joback Method
cpg	207.44	J/mol×K	490.53	Joback Method
cpg	219.64	J/mol×K	526.57	Joback Method
cpg	231.22	J/mol×K	562.60	Joback Method
cpg	242.18	J/mol×K	598.63	Joback Method
cpg	252.53	J/mol×K	634.66	Joback Method

dvisc	0.0133475	Pa×s	229.68	Joback Method
dvisc	0.0051931	Pa×s	261.14	Joback Method
dvisc	0.0024753	Pa×s	292.61	Joback Method
dvisc	0.0013624	Pa×s	324.07	Joback Method
dvisc	0.0008335	Pa×s	355.54	Joback Method
dvisc	0.0005523	Pa×s	387.00	Joback Method
dvisc	0.0003893	Pa×s	418.47	Joback Method

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=R142591&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
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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