

Ketene, diethyl acetal

Inchi:	InChI=1S/C6H12O2/c1-4-7-6(3)8-5-2/h3-5H2,1-2H3
InchiKey:	VTGIVYVOVVQLRL-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	C=C(OCC)OCC
Mol. weight [g/mol]:	116.16

Physical Properties

Property code	Value	Unit	Source
gf	-131.07	kJ/mol	Joback Method
hf	-315.97	kJ/mol	Joback Method
hfus	11.08	kJ/mol	Joback Method
hvap	33.18	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.531		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	378.08	K	Joback Method
tc	550.11	K	Joback Method
tf	186.12	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.57	J/molxK	378.08	Joback Method
cpg	200.04	J/molxK	406.75	Joback Method
cpg	209.27	J/molxK	435.42	Joback Method
cpg	218.27	J/molxK	464.10	Joback Method
cpg	227.03	J/molxK	492.77	Joback Method
cpg	235.54	J/molxK	521.44	Joback Method
cpg	243.79	J/molxK	550.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
mccvol:	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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