

«gamma»-methylen-«gamma»-butyrolactone

Inchi:	InChI=1S/C5H6O2/c1-4-2-3-5(6)7-4/h1-3H2
InchiKey:	SIFBVNDLLGPEKT-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	C=C1CCC(=O)O1
Mol. weight [g/mol]:	98.10

Physical Properties

Property code	Value	Unit	Source
gf	-120.15	kJ/mol	Joback Method
hf	-251.17	kJ/mol	Joback Method
hfus	7.90	kJ/mol	Joback Method
hvap	36.21	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	0.837		Crippen Method
mvol	73.590	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
tb	427.68	K	Joback Method
tc	650.12	K	Joback Method
tf	269.72	K	Joback Method
vc	0.270	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.40	J/mol×K	427.68	Joback Method
cpg	148.86	J/mol×K	464.75	Joback Method
cpg	157.98	J/mol×K	501.83	Joback Method
cpg	166.72	J/mol×K	538.90	Joback Method
cpg	175.09	J/mol×K	575.98	Joback Method
cpg	183.08	J/mol×K	613.05	Joback Method
cpg	190.66	J/mol×K	650.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=R492683&Units=SI

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
h vap:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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