ALPHA-METHYLENE-GAMMA-BUTYROLACTONE

Other names:	Dihydro-3-methylene-2(3H)-furanone
	Tulipalin A
	alpha-methylene-«gamma»-butyrolactone
	«alpha»-Methylene butyrolactone
	«alpha»-Methylene-«gamma»-butyrolactone
Inchi:	InChI=1S/C5H6O2/c1-4-2-3-7-5(4)6/h1-3H2
InchiKey:	GSLDEZOOOSBFGP-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	C=C1CCOC1=O
Mol. weight [g/mol]:	98.10

Physical Properties

Property code	Value	Unit	Source
hf	-231.22	kJ/mol	Cheméo Relay (1.0)
hfus	7.90	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
logp	0.489		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
tb	450.92	K	Cheméo Relay (1.0)

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	1.60	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C547659&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure