2-Butenoic acid, 4-methyl, «gamma»-lactone

Inchi: InChI=1S/C5H6O2/c1-4-2-5(6)7-3-4/h2H,3H2,1H3
InchiKey: ZZEYQBNQZKUWKY-UHFFFAOYSA-N
Formula: C5H6O2
SMILES: CC1=CC(=O)OC1
Mol. weight [g/mol]: 98.10

Physical Properties

Property code	Value	Unit	Source
hfus	9.89	kJ/mol	Joback Method
logp	0.489		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
ripol	1635.00		NIST Webbook
ripol	1635.00		NIST Webbook
tf	316.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.67	J/mol×K	432.66	Joback Method
cpg	149.00	J/mol×K	470.03	Joback Method
cpg	157.97	J/mol×K	507.41	Joback Method
cpg	166.57	J/mol×K	544.78	Joback Method
cpg	174.79	J/mol×K	582.15	Joback Method
cpg	182.62	J/mol×K	619.53	Joback Method
cpg	190.05	J/mol×K	656.90	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R595534&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tf:	Normal melting (fusion) point