«beta»-Methyl-«gamma»-octalactone

Inchi: InChI=1S/C9H16O2/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3
InchiKey: WNVCMFHPRIBNCW-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CCCCC1OC(=O)CC1C
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
hf	-484.43	kJ/mol	Cheméo Relay (1.0)
hfus	21.56	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Cheméo Relay (1.0)
logp	2.128		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
rinpol	1281.00		NIST Webbook
rinpol	1281.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1968.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.83	J/mol×K	510.70	Joback Method
cpg	340.60	J/mol×K	545.27	Joback Method
cpg	356.64	J/mol×K	579.83	Joback Method
cpg	371.95	J/mol×K	614.40	Joback Method
cpg	386.53	J/mol×K	648.97	Joback Method
cpg	400.37	J/mol×K	683.53	Joback Method
cpg	413.48	J/mol×K	718.10	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613637&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices