SPIRO[4.5]DECAN-2-ONE

Other names: Spiro[4,5]decan-2-one
Inchi: InChI=1S/C10H16O/c11-9-4-7-10(8-9)5-2-1-3-6-10/h1-8H2
InchiKey: DJHRXBYWKVQDJY-UHFFFAOYSA-N
Formula: C10H16O
SMILES: O=C1CCC2(CCCCC2)C1
Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
hf	-254.10	kJ/mol	Cheméo Relay (1.0)
hfus	1.67	kJ/mol	Joback Method
hvap	56.59	kJ/mol	Cheméo Relay (1.0)
logp	2.690		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
rinpol	1180.00		NIST Webbook
tb	497.93	K	Cheméo Relay (1.0)
tf	294.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.99	J/mol×K	531.49	Joback Method
cpg	344.73	J/mol×K	573.18	Joback Method
cpg	363.97	J/mol×K	614.87	Joback Method
cpg	381.88	J/mol×K	656.56	Joback Method
cpg	398.65	J/mol×K	698.25	Joback Method
cpg	414.43	J/mol×K	739.94	Joback Method
cpg	429.42	J/mol×K	781.63	Joback Method

Sources

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=C3643161&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point