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]: 152.23
CAS: 3643-16-1

Physical Properties

Property code	Value	Unit	Source
gf	-13.95	kJ/mol	Joback Method
hf	-230.89	kJ/mol	Joback Method
hfus	1.67	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.690		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1180.00		NIST Webbook
tb	531.49	K	Joback Method
tc	781.63	K	Joback Method
tf	320.62	K	Joback Method
vc	0.483	m3/kmol	Joback Method

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:	https://www.chemeo.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=C3643161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/79-675-6/Spiro-4-5-decan-2-one.pdf

Generated by Cheméo on 2024-10-12 05:53:43.363367447 +0000 UTC m=+3293286.000336699.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.