

Spiro[4.5]decan-7-one, 1,8-dimethyl-4-(1-methylethyl)-

Other names: 1-Isopropyl-4,8-dimethylspiro[4.5]decan-7-one

Inchi: InChI=1S/C15H26O/c1-10(2)13-6-5-12(4)15(13)8-7-11(3)14(16)9-15/h10-13H,5-9H2,1-4

InchiKey: HGEHVVBKUMPQRX-UHFFFAOYSA-N

Formula: C15H26O

SMILES: CC1CCC2(CC1=O)C(C)CCC2C(C)C

Mol. weight [g/mol]: 222.37

CAS: 39510-26-4

Physical Properties

Property code	Value	Unit	Source
gf	2.58	kJ/mol	Joback Method
hf	-400.39	kJ/mol	Joback Method
hfus	14.31	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	4.064		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1681.70		NIST Webbook
rinpol	1681.70		NIST Webbook
tb	631.44	K	Joback Method
tc	862.13	K	Joback Method
tf	349.25	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.44	J/molxK	631.44	Joback Method
cpg	611.29	J/molxK	669.89	Joback Method
cpg	634.74	J/molxK	708.34	Joback Method
cpg	656.91	J/molxK	746.79	Joback Method
cpg	677.92	J/molxK	785.24	Joback Method
cpg	697.92	J/molxK	823.68	Joback Method

Sources

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=C39510264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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