

endo-Tricyclo[6,2,1,0(2,6)]decan-8-one

Inchi:	InChI=1S/C10H14O/c11-10-5-6-4-9(10)8-3-1-2-7(6)8/h6-9H,1-5H2/t6?,7-,8-,9?/m1/s1
InchiKey:	OMIDXVJKZCPKEI-OMRMXDLSA-N
Formula:	C10H14O
SMILES:	O=C1CC2CC1C1CCCC21
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
gf	73.17	kJ/mol	Joback Method
hf	-195.53	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	41.70	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.012		Crippen Method
mcvol	120.750	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1821.00		NIST Webbook
tb	515.84	K	Joback Method
tc	746.98	K	Joback Method
tf	316.74	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.43	J/molxK	515.84	Joback Method
cpg	330.08	J/molxK	554.36	Joback Method
cpg	348.41	J/molxK	592.89	Joback Method
cpg	365.50	J/molxK	631.41	Joback Method
cpg	381.43	J/molxK	669.93	Joback Method
cpg	396.28	J/molxK	708.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R386266&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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