

endo-Tricyclo[6,2,1,0(2,6)]dec-3-en-8-one

Inchi:	InChI=1S/C10H12O/c11-10-5-6-4-9(10)8-3-1-2-7(6)8/h1-2,6-9H,3-5H2/t6?,7-,8-,9?/m1/s?
InchiKey:	BNISRVGIGGHBIM-OMRMXDLSA-N
Formula:	C10H12O
SMILES:	O=C1CC2CC1C1CC=CC21
Mol. weight [g/mol]:	148.20

Physical Properties

Property code	Value	Unit	Source
gf	103.13	kJ/mol	Joback Method
hf	-137.75	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	42.00	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.788		Crippen Method
mcvol	116.450	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
ripol	1828.00		NIST Webbook
tb	515.00	K	Joback Method
tc	748.55	K	Joback Method
tf	317.50	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.87	J/mol×K	515.00	Joback Method
cpg	311.24	J/mol×K	553.92	Joback Method
cpg	328.32	J/mol×K	592.85	Joback Method
cpg	344.19	J/mol×K	631.77	Joback Method
cpg	358.94	J/mol×K	670.70	Joback Method
cpg	372.66	J/mol×K	709.62	Joback Method
cpg	385.43	J/mol×K	748.55	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=R386162&Units=SI

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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