

Tuberolactone

Inchi:	InChI=1S/C10H14O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h3-5,8-9H,2,6-7H2,1H3/b4-3-
InchiKey:	VYPONAGZHAJHGT-ARJAWSKDSA-N
Formula:	C10H14O2
SMILES:	CCC=CCC1CC=CC(=O)O1
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
gf	-40.76	kJ/mol	Joback Method
hf	-290.11	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	47.29	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.214		Crippen Method
mvol	139.740	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1440.00		NIST Webbook
ripol	2320.00		NIST Webbook
tb	545.84	K	Joback Method
tc	769.63	K	Joback Method
tf	300.31	K	Joback Method
vc	0.522	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.90	J/mol×K	545.84	Joback Method
cpg	350.54	J/mol×K	583.14	Joback Method
cpg	366.25	J/mol×K	620.44	Joback Method
cpg	381.06	J/mol×K	657.74	Joback Method
cpg	394.97	J/mol×K	695.03	Joback Method
cpg	408.00	J/mol×K	732.33	Joback Method
cpg	420.17	J/mol×K	769.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229044&Units=SI
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

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

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