

Thuj-3-en-10-al

Inchi: InChI=1S/C10H14O/c1-7(2)10-4-3-8(6-11)9(10)5-10/h3-4,6-9H,5H2,1-2H3
InchiKey: UQLNH DYBGCTZNJ-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC(C)C12C=CC(C=O)C1C2
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	69.62	kJ/mol	Joback Method
hf	-142.31	kJ/mol	Joback Method
hfus	12.69	kJ/mol	Joback Method
h vap	42.84	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.034		Crippen Method
m cvol	127.310	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1184.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1188.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook

ripol	1642.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1642.00		NIST Webbook
tb	484.63	K	Joback Method
tc	694.53	K	Joback Method
tf	285.76	K	Joback Method
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.22	J/mol×K	484.63	Joback Method
cpg	315.15	J/mol×K	519.61	Joback Method
cpg	329.80	J/mol×K	554.60	Joback Method
cpg	343.33	J/mol×K	589.58	Joback Method
cpg	355.89	J/mol×K	624.56	Joback Method
cpg	367.61	J/mol×K	659.55	Joback Method
cpg	378.65	J/mol×K	694.53	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=R227206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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