

Pinol

Other names:	6,8-Epoxymenth-1-ene (Pinol) 4,7,7-trimethyl-6-oxabicyclo[3.2.1]oct-3-ene
Inchi:	InChI=1S/C10H16O/c1-7-4-5-8-6-9(7)11-10(8,2)3/h4,8-9H,5-6H2,1-3H3
InchiKey:	SKBXVAOMEVOTGJ-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CCC2CC1OC2(C)C
Mol. weight [g/mol]:	152.23
CAS:	2437-97-0

Physical Properties

Property code	Value	Unit	Source
gf	51.63	kJ/mol	Joback Method
hf	-207.24	kJ/mol	Joback Method
hfus	17.31	kJ/mol	Joback Method
hvap	42.03	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.520		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
tb	476.88	K	Joback Method
tc	693.43	K	Joback Method
tf	290.81	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.36	J/mol×K	476.88	Joback Method
cpg	324.50	J/mol×K	512.97	Joback Method

cpg	341.34	J/mol×K	549.06	Joback Method
cpg	357.01	J/mol×K	585.16	Joback Method
cpg	371.64	J/mol×K	621.25	Joback Method
cpg	385.38	J/mol×K	657.34	Joback Method
cpg	398.36	J/mol×K	693.43	Joback Method

Sources

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=C2437970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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