«alpha»-Thujenal

Inchi: InChI=1S/C10H14O/c1-7(2)10-4-3-8(6-11)9(10)5-10/h3,6-7,9H,4-5H2,1-2H3
InchiKey: YZNIFKFTGCAOST-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC(C)C12CC=C(C=O)C1C2
Mol. weight [g/mol]: 150.22
CAS: 57129-54-1

Physical Properties

Property code	Value	Unit	Source
gf	67.70	kJ/mol	Joback Method
hf	-133.44	kJ/mol	Joback Method
hfus	11.23	kJ/mol	Joback Method
hvap	43.81	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1189.80		NIST Webbook
rinpol	1189.80		NIST Webbook
tb	494.28	K	Joback Method
tc	705.65	K	Joback Method
tf	302.52	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.04	J/mol×K	494.28	Joback Method
cpg	314.06	J/mol×K	529.51	Joback Method
cpg	327.87	J/mol×K	564.74	Joback Method
cpg	340.62	J/mol×K	599.97	Joback Method
cpg	352.47	J/mol×K	635.20	Joback Method
cpg	363.57	J/mol×K	670.42	Joback Method
cpg	374.07	J/mol×K	705.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57129541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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