«gamma»-Terpinyl acetate

Other names:	«gamma»-Terpenyl acetate
	1-methyl-4-(1-methylethylidene)cyclohexyl acetate
Inchi:	InChI=1S/C12H20O2/c1-9(2)11-5-7-12(4,8-6-11)14-10(3)13/h5-8H2,1-4H3
InchiKey:	ZKKBZSOYCMSYRW-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC1(C)CCC(=C(C)C)CC1
Mol. weight [g/mol]:	196.29
CAS:	10235-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-127.89	kJ/mol	Joback Method
hf	-400.01	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.219		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1336.00		NIST Webbook
rinpol	1256.40		NIST Webbook
rinpol	1341.30		NIST Webbook
rinpol	1354.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1696.00		NIST Webbook
tb	576.56	K	Joback Method
tc	794.00	K	Joback Method
tf	324.84	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	433.75	J/mol×K	576.56	Joback Method
cpg	451.92	J/mol×K	612.80	Joback Method
cpg	469.07	J/mol×K	649.04	Joback Method
cpg	485.31	J/mol×K	685.28	Joback Method
cpg	500.74	J/mol×K	721.52	Joback Method
cpg	515.48	J/mol×K	757.76	Joback Method
cpg	529.62	J/mol×K	794.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10235639&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
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
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

Latest version available from:
https://www.chemeo.com/cid/85-046-7/gamma-Terpinyl-acetate.pdf
Generated by Cheméo on 2024-04-27 17:38:50.009757095 +0000 UTC m=+16528778.930334417.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.