

Cyclohexanol, 3,3,5-trimethyl-, acetate, cis-

Other names:	3,3,5-Trimethylcyclohexyl acetate cis-3,3,5-trimethylcyclohexyl acetate
Inchi:	InChI=1S/C11H20O2/c1-8-5-10(13-9(2)12)7-11(3,4)6-8/h8,10H,5-7H2,1-4H3
InchiKey:	OIVWFAFCHQDCCG-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CC(=O)OC1CC(C)CC(C)(C)C1
Mol. weight [g/mol]:	184.28
CAS:	24691-16-5

Physical Properties

Property code	Value	Unit	Source
gf	-188.64	kJ/mol	Joback Method
hf	-486.29	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.764		Crippen Method
mvol	162.430	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
tb	537.82	K	Joback Method
tc	747.99	K	Joback Method
tf	308.69	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.89	J/molxK	537.82	Joback Method
cpg	424.16	J/molxK	572.85	Joback Method
cpg	442.41	J/molxK	607.88	Joback Method
cpg	459.70	J/molxK	642.90	Joback Method
cpg	476.12	J/molxK	677.93	Joback Method

cpg	491.75	J/mol×K	712.96	Joback Method
cpg	506.66	J/mol×K	747.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24691165&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

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

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