Cyclopentanol, 2,4,4-trimethyl-

Other names: 2,4,4-Trimethylcyclopentanol
Inchi: InChI=1S/C8H16O/c1-6-4-8(2,3)5-7(6)9/h6-7,9H,4-5H2,1-3H3
InchiKey: QIXDCVATINBRLV-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CC1CC(C)(C)CC1O
Mol. weight [g/mol]: 128.21
CAS: 56470-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-104.70	kJ/mol	Joback Method
hf	-325.64	kJ/mol	Joback Method
hfus	10.34	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.803		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
ripol	1365.00		NIST Webbook
tb	480.80	K	Joback Method
tc	671.51	K	Joback Method
tf	267.06	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.69	J/mol×K	480.80	Joback Method
cpg	291.36	J/mol×K	512.58	Joback Method
cpg	305.19	J/mol×K	544.37	Joback Method
cpg	318.26	J/mol×K	576.15	Joback Method
cpg	330.63	J/mol×K	607.94	Joback Method
cpg	342.39	J/mol×K	639.72	Joback Method
cpg	353.59	J/mol×K	671.51	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=C56470838&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume