

1,2,3-Trimethylcyclopentadiene

Inchi:	InChI=1S/C8H12/c1-6-4-5-7(2)8(6)3/h4H,5H2,1-3H3
InchiKey:	WFZFDWAAGYEXOS-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	CC1=CCC(C)=C1C
Mol. weight [g/mol]:	108.18
CAS:	3853-27-8

Physical Properties

Property code	Value	Unit	Source
gf	91.77	kJ/mol	Joback Method
hf	-46.48	kJ/mol	Joback Method
hfus	10.62	kJ/mol	Joback Method
hvap	36.54	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.673		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	415.65	K	Joback Method
tc	617.53	K	Joback Method
tf	234.14	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.78	J/molxK	415.65	Joback Method
cpg	248.07	J/molxK	583.88	Joback Method
cpg	238.08	J/molxK	550.23	Joback Method
cpg	227.57	J/molxK	516.59	Joback Method
cpg	216.53	J/molxK	482.94	Joback Method
cpg	204.94	J/molxK	449.30	Joback Method
cpg	257.57	J/molxK	617.53	Joback Method
dvisc	0.0002414	Paxs	415.65	Joback Method
dvisc	0.0002848	Paxs	385.40	Joback Method

dvisc	0.0003458	Paxs	355.15	Joback Method
dvisc	0.0004352	Paxs	324.89	Joback Method
dvisc	0.0005741	Paxs	294.64	Joback Method
dvisc	0.0008071	Paxs	264.39	Joback Method
dvisc	0.0012389	Paxs	234.14	Joback Method

Sources

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=C3853278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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