

1-trans-2-cis-4-Trimethylcyclopentane

Inchi:	InChI=1S/C8H16/c1-6-4-7(2)8(3)5-6/h6-8H,4-5H2,1-3H3/t7-,8-/m1/s1
InchiKey:	PNUFYSGVPVMNRN-HTQZYQBOSA-N
Formula:	C8H16
SMILES:	CC1CC(C)C(C)C1
Mol. weight [g/mol]:	112.21

Physical Properties

Property code	Value	Unit	Source
gf	37.61	kJ/mol	Joback Method
hf	-188.65	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	33.04	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.688		Crippen Method
mvol	112.720	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	738.00		NIST Webbook
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tb	388.38	K	Joback Method
tc	579.97	K	Joback Method
tf	182.34	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.62	J/molxK	388.38	Joback Method
cpg	291.26	J/molxK	548.04	Joback Method
cpg	277.08	J/molxK	516.11	Joback Method
cpg	262.24	J/molxK	484.17	Joback Method
cpg	246.72	J/molxK	452.24	Joback Method
cpg	230.52	J/molxK	420.31	Joback Method
cpg	304.79	J/molxK	579.97	Joback Method
dvisc	0.0002619	Paxs	388.38	Joback Method

dvisc	0.0002952	Paxs	354.04	Joback Method
dvisc	0.0003414	Paxs	319.70	Joback Method
dvisc	0.0004089	Paxs	285.36	Joback Method
dvisc	0.0005145	Paxs	251.02	Joback Method
dvisc	0.0006962	Paxs	216.68	Joback Method
dvisc	0.0010560	Paxs	182.34	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R633913&Units=SI

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

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