cis,trans,trans-1,2,4-Trimethylcyclohexane

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
mcvol	112.720	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
tb	388.38	K	Joback Method
tc	579.97	K	Joback Method
tf	182.34	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.62	J/mol×K	388.38	Joback Method
cpg	230.52	J/mol×K	420.31	Joback Method
cpg	246.72	J/mol×K	452.24	Joback Method
cpg	262.24	J/mol×K	484.17	Joback Method
cpg	277.08	J/mol×K	516.11	Joback Method
cpg	291.26	J/mol×K	548.04	Joback Method
cpg	304.79	J/mol×K	579.97	Joback Method
dvisc	0.0010560	Pa×s	182.34	Joback Method

dvisc	0.0006962	Pa×s	216.68	Joback Method
dvisc	0.0005145	Pa×s	251.02	Joback Method
dvisc	0.0004089	Pa×s	285.36	Joback Method
dvisc	0.0003414	Pa×s	319.70	Joback Method
dvisc	0.0002952	Pa×s	354.04	Joback Method
dvisc	0.0002619	Pa×s	388.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R634129&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
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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