

e,e-3,5-Dimethylcyclohexanol (a)

Inchi:	InChI=1S/C8H16O/c1-6-3-7(2)5-8(9)4-6/h6-9H,3-5H2,1-2H3
InchiKey:	WIYNOPYNRFPWNB-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CC1CC(C)CC(O)C1
Mol. weight [g/mol]:	128.21

Physical Properties

Property code	Value	Unit	Source
gf	-111.31	kJ/mol	Joback Method
hf	-347.04	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	49.89	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.803		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinsol	1025.00		NIST Webbook
tb	484.83	K	Joback Method
tc	674.82	K	Joback Method
tf	239.64	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.01	J/molxK	484.83	Joback Method
cpg	291.52	J/molxK	516.49	Joback Method
cpg	306.35	J/molxK	548.16	Joback Method
cpg	320.50	J/molxK	579.82	Joback Method
cpg	334.00	J/molxK	611.49	Joback Method
cpg	346.84	J/molxK	643.15	Joback Method
cpg	359.03	J/molxK	674.82	Joback Method
dvisc	0.0327662	Paxs	239.64	Joback Method
dvisc	0.0075606	Paxs	280.50	Joback Method

dvisc	0.0025331	Paxs	321.37	Joback Method
dvisc	0.0010862	Paxs	362.24	Joback Method
dvisc	0.0005530	Paxs	403.10	Joback Method
dvisc	0.0003188	Paxs	443.97	Joback Method
dvisc	0.0002017	Paxs	484.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R96212&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
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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