e,a-2,5-Dimethylcyclohexanol, (e)

Inchi: InChI=1S/C8H16O/c1-6-3-4-7(2)8(9)5-6/h6-9H,3-5H2,1-2H3/t6-,7+,8+/m0/s1
InchiKey: RUADGOLRFXTMCY-XLPZGREQSA-N
Formula: C8H16O
SMILES: CC1CCC(C)C(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
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
tb	484.83	K	Joback Method
tc	674.82	K	Joback Method
tf	239.64	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.01	J/mol×K	484.83	Joback Method
cpg	291.52	J/mol×K	516.49	Joback Method
cpg	306.35	J/mol×K	548.16	Joback Method
cpg	320.50	J/mol×K	579.82	Joback Method
cpg	334.00	J/mol×K	611.49	Joback Method
cpg	346.84	J/mol×K	643.15	Joback Method
cpg	359.03	J/mol×K	674.82	Joback Method
dvisc	0.0327662	Pa×s	239.64	Joback Method

dvisc	0.0075606	Pa×s	280.50	Joback Method
dvisc	0.0025331	Pa×s	321.37	Joback Method
dvisc	0.0010862	Pa×s	362.24	Joback Method
dvisc	0.0005530	Pa×s	403.10	Joback Method
dvisc	0.0003188	Pa×s	443.97	Joback Method
dvisc	0.0002017	Pa×s	484.83	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=R96141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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