

d14 Cymene

Inchi:	InChI=1S/C10H14/c1-8(2)10-6-4-9(3)5-7-10/h4-8H,1-3H3/i1D3,2D3,3D3,4D,5D,6D,7D,8D
InchiKey:	HFPZCAJZSCWRBC-UYAILFBOSA-N
Formula:	C10D14
SMILES:	Cc1ccc(C(C)C)cc1
Mol. weight [g/mol]:	148.30

Physical Properties

Property code	Value	Unit	Source
gf	133.66	kJ/mol	Joback Method
hf	-29.95	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.118		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rmpol	1004.20		NIST Webbook
tb	459.42	K	Joback Method
tc	670.22	K	Joback Method
tf	226.40	K	Joback Method
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.41	J/molxK	459.42	Joback Method
cpg	325.13	J/molxK	635.09	Joback Method
cpg	313.10	J/molxK	599.96	Joback Method
cpg	300.33	J/molxK	564.82	Joback Method
cpg	286.82	J/molxK	529.69	Joback Method
cpg	272.52	J/molxK	494.55	Joback Method
cpg	336.48	J/molxK	670.22	Joback Method
dvisc	0.0002060	Paxs	459.42	Joback Method
dvisc	0.0002660	Paxs	420.58	Joback Method

dvisc	0.0003618	Paxs	381.75	Joback Method
dvisc	0.0005277	Paxs	342.91	Joback Method
dvisc	0.0008475	Paxs	304.07	Joback Method
dvisc	0.0015637	Paxs	265.24	Joback Method
dvisc	0.0035598	Paxs	226.40	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=R327767&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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