1-Acenaphthenol

Other names:	Acenaphthenol-1
	1-Acenaphthylenol, 1,2-dihydro-
	7-Acenaphthenol
	acenaphthen-1-ol
Inchi:	InChI=1S/C12H10O/c13-11-7-9-5-1-3-8-4-2-6-10(11)12(8)9/h1-6,11,13H,7H2
InchiKey:	MXUCIEHYJYRTLT-UHFFFAOYSA-N
Formula:	C12H10O
SMILES:	OC1Cc2cccc3cccc1c23
Mol. weight [g/mol]:	170.21
CAS:	6306-07-6

Physical Properties

Property code	Value	Unit	Source
gf	185.99	kJ/mol	Joback Method
hf	40.38	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.429		Crippen Method
mcvol	131.730	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
rinpol	1625.00		NIST Webbook
tb	624.23	K	Joback Method
tc	845.25	K	Joback Method
tf	421.65 ± 1.50	K	NIST Webbook
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.58	J/mol×K	624.23	Joback Method
cpg	341.96	J/mol×K	661.07	Joback Method
cpg	352.49	J/mol×K	697.90	Joback Method
cpg	362.28	J/mol×K	734.74	Joback Method

cpg	371.42	J/mol×K	771.57	Joback Method
cpg	380.01	J/mol×K	808.41	Joback Method
cpg	388.15	J/mol×K	845.25	Joback Method
dvisc	0.0025801	Pa×s	391.44	Joback Method
dvisc	0.0016037	Pa×s	430.24	Joback Method
dvisc	0.0010784	Pa×s	469.04	Joback Method
dvisc	0.0007705	Pa×s	507.84	Joback Method
dvisc	0.0005774	Pa×s	546.63	Joback Method
dvisc	0.0004496	Pa×s	585.43	Joback Method
dvisc	0.0003611	Pa×s	624.23	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6306076&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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