4-Acenaphthylenol

Inchi: InChI=1S/C12H8O/c13-11-6-9-3-1-2-8-4-5-10(7-11)12(8)9/h1-7,13H
InchiKey: JKRUSJXWUPHOHB-UHFFFAOYSA-N
Formula: C12H8O
SMILES: Oc1cc2c3c(cccc3c1)C=C2
Mol. weight [g/mol]: 168.19

Physical Properties

Property code	Value	Unit	Source
gf	205.86	kJ/mol	Joback Method
hf	93.42	kJ/mol	Joback Method
hfus	23.29	kJ/mol	Joback Method
hvap	60.90	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.029		Crippen Method
mcvol	127.430	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
rinpol	264.80		NIST Webbook
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tb	616.50	K	Joback Method
tc	870.55	K	Joback Method
tf	447.34	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.25	J/mol×K	616.50	Joback Method
cpg	351.70	J/mol×K	828.21	Joback Method
cpg	343.69	J/mol×K	785.87	Joback Method
cpg	335.37	J/mol×K	743.53	Joback Method
cpg	326.50	J/mol×K	701.18	Joback Method
cpg	316.87	J/mol×K	658.84	Joback Method
cpg	359.61	J/mol×K	870.55	Joback Method
dvisc	0.0001414	Pa×s	616.50	Joback Method

dvisc	0.0001787	Pa×s	588.31	Joback Method
dvisc	0.0002312	Pa×s	560.11	Joback Method
dvisc	0.0003073	Pa×s	531.92	Joback Method
dvisc	0.0004218	Pa×s	503.73	Joback Method
dvisc	0.0006011	Pa×s	475.53	Joback Method
dvisc	0.0008956	Pa×s	447.34	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=R572402&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