1(2H)-Acenaphthylenone

Other names:	1-Acenaphthenone
	Acenaphthenone
	2-Acenaphthenone
	NSC 18756
	1-Acenaphenone
Inchi:	InChI=1S/C12H8O/c13-11-7-9-5-1-3-8-4-2-6-10(11)12(8)9/h1-6H,7H2
InchiKey:	JBXIOAKUBCTDES-UHFFFAOYSA-N
Formula:	C12H8O
SMILES:	O=C1Cc2cccc3cccc1c23
Mol. weight [g/mol]:	168.19
CAS:	2235-15-6

Physical Properties

Property code	Value	Unit	Source
gf	207.93	kJ/mol	Joback Method
hf	75.25	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	51.84	kJ/mol	Joback Method
ie	8.29	eV	NIST Webbook
log10ws	-3.80		Crippen Method
logp	2.579		Crippen Method
mcvol	127.430	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	280.60		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	280.60		NIST Webbook
rinpol	1589.00		NIST Webbook
tb	604.54	K	Joback Method
tc	860.23	K	Joback Method
tf	403.08	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.18	J/mol×K	604.54	Joback Method
cpg	315.28	J/mol×K	647.16	Joback Method
cpg	327.32	J/mol×K	689.77	Joback Method
cpg	338.43	J/mol×K	732.39	Joback Method
cpg	348.70	J/mol×K	775.00	Joback Method
cpg	358.24	J/mol×K	817.62	Joback Method
cpg	367.17	J/mol×K	860.23	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=C2235156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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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