

Acenaphthylene-1-carboxaldehyde

Inchi:	InChI=1S/C13H8O/c14-8-11-7-10-5-1-3-9-4-2-6-12(11)13(9)10/h1-8H
InchiKey:	DJGQYTUXTCURSC-UHFFFAOYSA-N
Formula:	C13H8O
SMILES:	O=CC1=Cc2cccc3cccc1c23
Mol. weight [g/mol]:	180.20

Physical Properties

Property code	Value	Unit	Source
gf	259.75	kJ/mol	Joback Method
hf	153.04	kJ/mol	Joback Method
hfus	21.99	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.893		Crippen Method
mcvol	137.220	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	303.40		NIST Webbook
rinpol	303.40		NIST Webbook
tb	612.40	K	Joback Method
tc	853.95	K	Joback Method
tf	401.41	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.80	J/mol×K	612.40	Joback Method
cpg	367.92	J/mol×K	813.69	Joback Method
cpg	359.70	J/mol×K	773.43	Joback Method
cpg	350.90	J/mol×K	733.17	Joback Method
cpg	341.41	J/mol×K	692.92	Joback Method
cpg	331.08	J/mol×K	652.66	Joback Method
cpg	375.71	J/mol×K	853.95	Joback Method
dvisc	0.0010285	Pa×s	612.40	Joback Method

dvisc	0.0011061	Pa×s	577.24	Joback Method
dvisc	0.0012010	Pa×s	542.07	Joback Method
dvisc	0.0013189	Pa×s	506.91	Joback Method
dvisc	0.0014688	Pa×s	471.74	Joback Method
dvisc	0.0016643	Pa×s	436.58	Joback Method
dvisc	0.0019277	Pa×s	401.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312582&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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