1-Naphthalenecarboxaldehyde, 4-methoxy-

Other names: 4-Methoxy-1-naphthaldehyde
4-Methoxy-1-naphthalenecarboxaldehyde
1-Naphthaldehyde, 4-methoxy-
Inchi: InChI=1S/C12H10O2/c1-14-12-7-6-9(8-13)10-4-2-3-5-11(10)12/h2-8H,1H3
InchiKey: MVXMNHYVCLMLDD-UHFFFAOYSA-N
Formula: C12H10O2
SMILES: COc1ccc(C=O)c2ccccc12
Mol. weight [g/mol]: 186.21
CAS: 15971-29-6

Physical Properties

Property code	Value	Unit	Source
gf	45.44	kJ/mol	Joback Method
hf	-104.15	kJ/mol	Joback Method
hfus	20.60	kJ/mol	Joback Method
hvap	56.68	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.661		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
tb	600.66	K	Joback Method
tc	831.51	K	Joback Method
tf	373.39	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.73	J/mol×K	600.66	Joback Method
cpg	349.41	J/mol×K	639.13	Joback Method
cpg	361.23	J/mol×K	677.61	Joback Method
cpg	372.23	J/mol×K	716.08	Joback Method

cpg	382.45	J/mol×K	754.56	Joback Method
cpg	391.93	J/mol×K	793.03	Joback Method
cpg	400.73	J/mol×K	831.51	Joback Method
dvisc	0.0013087	Pa×s	373.39	Joback Method
dvisc	0.0009292	Pa×s	411.27	Joback Method
dvisc	0.0006990	Pa×s	449.15	Joback Method
dvisc	0.0005496	Pa×s	487.03	Joback Method
dvisc	0.0004474	Pa×s	524.90	Joback Method
dvisc	0.0003744	Pa×s	562.78	Joback Method
dvisc	0.0003205	Pa×s	600.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	485.20	K	5.30	NIST Webbook

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=C15971296&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume