

1-Naphthalenecarboxaldehyde, 2-methoxy-

Other names:	2-Methoxy-1-naphthaldehyde 2-Methoxy-1-naphthalenecarboxaldehyde 1-Naphthaldehyde, 2-methoxy-
Inchi:	InChI=1S/C12H10O2/c1-14-12-7-6-9-4-2-3-5-10(9)11(12)8-13/h2-8H,1H3
InchiKey:	YIQGLTKAOHRZOL-UHFFFAOYSA-N
Formula:	C12H10O2
SMILES:	COc1ccc2ccccc2c1C=O
Mol. weight [g/mol]:	186.21
CAS:	5392-12-1

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	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook
tb	600.66	K	Joback Method
tc	831.51	K	Joback Method
tf	373.39	K	Joback Method
vc	0.556	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

cpg	382.45	J/molxK	754.56	Joback Method
cpg	391.93	J/molxK	793.03	Joback Method
cpg	400.73	J/molxK	831.51	Joback Method
dvisc	0.0013087	Paxs	373.39	Joback Method
dvisc	0.0009292	Paxs	411.27	Joback Method
dvisc	0.0006990	Paxs	449.15	Joback Method
dvisc	0.0005496	Paxs	487.03	Joback Method
dvisc	0.0004474	Paxs	524.90	Joback Method
dvisc	0.0003744	Paxs	562.78	Joback Method
dvisc	0.0003205	Paxs	600.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	478.20	K	2.40	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=C5392121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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