4-Methyl-1-naphthaldehyde

Inchi: InChI=1S/C12H10O/c1-9-6-7-10(8-13)12-5-3-2-4-11(9)12/h2-8H,1H3
InchiKey: LANRGTXVAPBSIA-UHFFFAOYSA-N
Formula: C12H10O
SMILES: Cc1ccc(C=O)c2ccccc12
Mol. weight [g/mol]: 170.21

Physical Properties

Property code	Value	Unit	Source
af	0.4904		Cheméo Relay (1.0)
hfus	19.41	kJ/mol	Joback Method
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-3.38		Cheméo Relay (1.0)
logp	2.961		Crippen Method
mcvol	138.290	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	582.01	K	Cheméo Relay (1.0)
tc	858.57	K	Cheméo Relay (1.0)
tf	333.66	K	Cheméo Relay (1.0)
vc	0.505	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.45	J/mol×K	578.24	Joback Method
cpg	326.42	J/mol×K	617.27	Joback Method
cpg	338.45	J/mol×K	656.29	Joback Method
cpg	349.59	J/mol×K	695.32	Joback Method
cpg	359.93	J/mol×K	734.35	Joback Method
cpg	369.51	J/mol×K	773.38	Joback Method
cpg	378.41	J/mol×K	812.40	Joback Method
dvisc	0.0015729	Pa×s	351.16	Joback Method
dvisc	0.0011075	Pa×s	389.01	Joback Method
dvisc	0.0008298	Pa×s	426.85	Joback Method
dvisc	0.0006517	Pa×s	464.70	Joback Method

dvisc	0.0005308	Pa×s	502.55	Joback Method
dvisc	0.0004449	Pa×s	540.39	Joback Method
dvisc	0.0003817	Pa×s	578.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.20	K	1.70	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33738486&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion 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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume