1-Naphthalenecarboxylic acid, methyl ester

Other names:	1-Naphthoic acid, methyl ester
	Methyl 1-naphthalenecarboxylate
	Methyl 1-naphthoate
	1-(Methoxycarbonyl)naphthalene
Inchi:	InChI=1S/C12H10O2/c1-14-12(13)11-8-4-6-9-5-2-3-7-10(9)11/h2-8H,1H3
InchiKey:	HMRROBKAACRWBP-UHFFFAOYSA-N
Formula:	C12H10O2
SMILES:	COC(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	186.21
CAS:	2459-24-7

Physical Properties

Property code	Value	Unit	Source
gf	25.67	kJ/mol	Joback Method
hf	-119.68	kJ/mol	Joback Method
hfus	20.29	kJ/mol	Joback Method
hvap	56.04	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.626		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	276.70		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	600.89	K	Joback Method
tc	836.14	K	Joback Method
tf	368.80	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.63	J/mol×K	600.89	Joback Method

cpg	349.90	J/mol×K	640.10	Joback Method
cpg	362.21	J/mol×K	679.31	Joback Method
cpg	373.60	J/mol×K	718.51	Joback Method
cpg	384.14	J/mol×K	757.72	Joback Method
cpg	393.88	J/mol×K	796.93	Joback Method
cpg	402.88	J/mol×K	836.14	Joback Method
dvisc	0.0014170	Pa×s	368.80	Joback Method
dvisc	0.0009648	Pa×s	407.48	Joback Method
dvisc	0.0007022	Pa×s	446.16	Joback Method
dvisc	0.0005377	Pa×s	484.85	Joback Method
dvisc	0.0004282	Pa×s	523.53	Joback Method
dvisc	0.0003519	Pa×s	562.21	Joback Method
dvisc	0.0002966	Pa×s	600.89	Joback Method

Sources

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=C2459247&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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