2-Naphthalenecarboxylic acid, methyl ester

Other names: 2-Naphthoic acid, methyl ester
Methyl 2-naphthalenecarboxylate
Methyl 2-naphthoate
Inchi: InChI=1S/C12H10O2/c1-14-12(13)11-7-6-9-4-2-3-5-10(9)8-11/h2-8H,1H3
InchiKey: IODOXLXFXNATGI-UHFFFAOYSA-N
Formula: C12H10O2
SMILES: COC(=O)c1ccc2ccccc2c1
Mol. weight [g/mol]: 186.21
CAS: 2459-25-8

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	1651.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	279.47		NIST Webbook
rinpol	279.47		NIST Webbook
tb	600.89	K	Joback Method
tc	836.14	K	Joback Method
tf	350.00 ± 0.10	K	NIST Webbook
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.88	J/mol×K	836.14	Joback Method
cpg	393.88	J/mol×K	796.93	Joback Method

cpg	384.14	J/mol×K	757.72	Joback Method
cpg	373.60	J/mol×K	718.51	Joback Method
cpg	362.21	J/mol×K	679.31	Joback Method
cpg	349.90	J/mol×K	640.10	Joback Method
cpg	336.63	J/mol×K	600.89	Joback Method
dvisc	0.0014170	Pa×s	368.80	Joback Method
dvisc	0.0002966	Pa×s	600.89	Joback Method
dvisc	0.0003519	Pa×s	562.21	Joback Method
dvisc	0.0004282	Pa×s	523.53	Joback Method
dvisc	0.0005377	Pa×s	484.85	Joback Method
dvisc	0.0007022	Pa×s	446.16	Joback Method
dvisc	0.0009648	Pa×s	407.48	Joback Method
hfust	27.10	kJ/mol	350.20	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2459258&Units=SI

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
hfust: Enthalpy of fusion at a given temperature
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