1-Naphthalenecarboxylic acid, ethyl ester

Other names: 1-Naphthoic acid, ethyl ester
Ethyl 1-naphthoate
Ethyl «alpha»-naphthoate
Inchi: InChI=1S/C13H12O2/c1-2-15-13(14)12-9-5-7-10-6-3-4-8-11(10)12/h3-9H,2H2,1H3
InchiKey: XCTLDQQOHIEUCJ-UHFFFAOYSA-N
Formula: C13H12O2
SMILES: CCOC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 200.23
CAS: 3007-97-4

Physical Properties

Property code	Value	Unit	Source
gf	34.09	kJ/mol	Joback Method
hf	-140.32	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	58.27	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.017		Crippen Method
mcvol	158.250	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	623.77	K	Joback Method
tc	854.32	K	Joback Method
tf	380.07	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.57	J/mol×K	623.77	Joback Method
cpg	398.55	J/mol×K	662.20	Joback Method
cpg	411.55	J/mol×K	700.62	Joback Method
cpg	423.62	J/mol×K	739.05	Joback Method
cpg	434.81	J/mol×K	777.47	Joback Method
cpg	445.18	J/mol×K	815.90	Joback Method

cpg	454.78	J/mol×K	854.32	Joback Method
dvisc	0.0014189	Pa×s	380.07	Joback Method
dvisc	0.0009480	Pa×s	420.69	Joback Method
dvisc	0.0006800	Pa×s	461.30	Joback Method
dvisc	0.0005147	Pa×s	501.92	Joback Method
dvisc	0.0004062	Pa×s	542.54	Joback Method
dvisc	0.0003313	Pa×s	583.15	Joback Method
dvisc	0.0002775	Pa×s	623.77	Joback Method

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=C3007974&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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume