

Ethyl «beta»-naphthoate

Other names:	Ethyl 2-naphthoate 2-Naphthalenecarboxylic acid, ethyl ester
Inchi:	InChI=1S/C13H12O2/c1-2-15-13(14)12-8-7-10-5-3-4-6-11(10)9-12/h3-9H,2H2,1H3
InchiKey:	HQKSINSCHCDMLS-UHFFFAOYSA-N
Formula:	C13H12O2
SMILES:	CCOC(=O)c1ccc2ccccc2c1
Mol. weight [g/mol]:	200.23
CAS:	3007-91-8

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
mvol	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	m ³ /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	Paxs	380.07	Joback Method
dvisc	0.0009480	Paxs	420.69	Joback Method
dvisc	0.0006800	Paxs	461.30	Joback Method
dvisc	0.0005147	Paxs	501.92	Joback Method
dvisc	0.0004062	Paxs	542.54	Joback Method
dvisc	0.0003313	Paxs	583.15	Joback Method
dvisc	0.0002775	Paxs	623.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	497.20	K	9.90	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=C3007918&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
mccvol:	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

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