

1-Naphthaleneacetic acid, methyl ester

Other names:	«alpha»-Naphthaleneacetic acid methyl ester «alpha»-Naphthylacetic acid methyl ester Hormonit Kartofin Methyl «alpha»-naphthylacetate Methyl 1-naphthaleneacetate Methyl 1-naphthylacetate 1-Naphthylacetic acid methyl ester Latka M-1 M 1 Methylester kyseliny 1-naftyloctove Methyl-1-naphtaleneacetic acid M 1 (Growth regulator) Methyl 1-naphthalenylacetate NSC 122030
Inchi:	InChI=1S/C13H12O2/c1-15-13(14)9-11-7-4-6-10-5-2-3-8-12(10)11/h2-8H,9H2,1H3
InchiKey:	YGGXZTQSGNFKPJ-UHFFFAOYSA-N
Formula:	C13H12O2
SMILES:	COC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]:	200.23
CAS:	2876-78-0

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	-3.36		Crippen Method
logp	2.555		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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.57	J/molxK	623.77	Joback Method
cpg	398.55	J/molxK	662.20	Joback Method
cpg	411.55	J/molxK	700.62	Joback Method
cpg	423.62	J/molxK	739.05	Joback Method
cpg	434.81	J/molxK	777.47	Joback Method
cpg	445.18	J/molxK	815.90	Joback Method
cpg	454.78	J/molxK	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	434.20	K	0.70	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C2876780&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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