

2-Naphthaleneacetic acid, ethyl ester

Other names:	Ethyl (2-naphthyl)acetate
Inchi:	InChI=1S/C14H14O2/c1-2-16-14(15)10-11-7-8-12-5-3-4-6-13(12)9-11/h3-9H,2,10H2,11H3
InchiKey:	PZNMRIQALHUBSJ-UHFFFAOYSA-N
Formula:	C14H14O2
SMILES:	CCOC(=O)Cc1ccc2ccccc2c1
Mol. weight [g/mol]:	214.26
CAS:	2876-70-2

Physical Properties

Property code	Value	Unit	Source
gf	42.51	kJ/mol	Joback Method
hf	-160.96	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	60.49	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.945		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
tb	646.65	K	Joback Method
tc	872.78	K	Joback Method
tf	391.34	K	Joback Method
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.01	J/molxK	646.65	Joback Method
cpg	497.48	J/molxK	835.09	Joback Method
cpg	486.57	J/molxK	797.41	Joback Method
cpg	474.83	J/molxK	759.72	Joback Method
cpg	462.19	J/molxK	722.03	Joback Method
cpg	448.60	J/molxK	684.34	Joback Method
cpg	507.61	J/molxK	872.78	Joback Method
dvisc	0.0002573	Paxs	646.65	Joback Method

dvisc	0.0003090	Paxs	604.10	Joback Method
dvisc	0.0003815	Paxs	561.55	Joback Method
dvisc	0.0004877	Paxs	519.00	Joback Method
dvisc	0.0006514	Paxs	476.44	Joback Method
dvisc	0.0009208	Paxs	433.89	Joback Method
dvisc	0.0014034	Paxs	391.34	Joback Method

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=C2876702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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