HEXYL 2-(1-NAPHTHYL)ACETATE

Other names: 1-naphthaleneacetic acid, hexyl ester
Inchi: InChI=1S/C18H22O2/c1-2-3-4-7-13-20-18(19)14-16-11-8-10-15-9-5-6-12-17(15)16/h5-6,
InchiKey: AIRQXTVJFPUCNR-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: CCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
af	0.7539		Cheméo Relay (1.0)
hf	-340.64	kJ/mol	Cheméo Relay (1.0)
hfus	35.83	kJ/mol	Joback Method
hvap	94.50	kJ/mol	Cheméo Relay (1.0)
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-5.00		Cheméo Relay (1.0)
logp	4.506		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
tb	646.23	K	Cheméo Relay (1.0)
tc	873.97	K	Cheméo Relay (1.0)
tf	304.30	K	Cheméo Relay (1.0)
vc	0.846	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.16	J/mol×K	738.17	Joback Method
cpg	728.02	J/mol×K	950.21	Joback Method
cpg	716.40	J/mol×K	914.87	Joback Method
cpg	703.99	J/mol×K	879.53	Joback Method
cpg	690.72	J/mol×K	844.19	Joback Method
cpg	676.53	J/mol×K	808.85	Joback Method
cpg	661.36	J/mol×K	773.51	Joback Method
dvisc	0.0003617	Pa×s	587.29	Joback Method

dvisc	0.0001767	Pa×s	738.17	Joback Method
dvisc	0.0002167	Pa×s	687.88	Joback Method
dvisc	0.0002744	Pa×s	637.59	Joback Method
dvisc	0.0012149	Pa×s	436.42	Joback Method
dvisc	0.0005022	Pa×s	537.00	Joback Method
dvisc	0.0007463	Pa×s	486.71	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2876735&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.