1-naphthaleneacetic acid, pentyl ester

Inchi: InChI=1S/C17H20O2/c1-2-3-6-12-19-17(18)13-15-10-7-9-14-8-4-5-11-16(14)15/h4-5,7-1
InchiKey: WTHHZUCMGNXCPB-UHFFFAOYSA-N
Formula: C17H20O2
SMILES: CCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 256.34
CAS: 2876-74-6

Physical Properties

Property code	Value	Unit	Source
af	0.7120		Cheméo Relay (1.0)
hf	-319.55	kJ/mol	Cheméo Relay (1.0)
hfus	33.24	kJ/mol	Joback Method
hvap	90.46	kJ/mol	Cheméo Relay (1.0)
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-4.61		Cheméo Relay (1.0)
logp	4.116		Crippen Method
mcvol	214.610	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
tb	634.81	K	Cheméo Relay (1.0)
tc	865.00	K	Cheméo Relay (1.0)
tf	302.59	K	Cheméo Relay (1.0)
vc	0.791	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.52	J/mol×K	715.29	Joback Method
cpg	606.42	J/mol×K	751.11	Joback Method
cpg	621.28	J/mol×K	786.94	Joback Method
cpg	635.17	J/mol×K	822.76	Joback Method
cpg	648.14	J/mol×K	858.59	Joback Method
cpg	660.26	J/mol×K	894.41	Joback Method
cpg	671.58	J/mol×K	930.24	Joback Method
dvisc	0.0012762	Pa×s	425.15	Joback Method

dvisc	0.0007962	Pa×s	473.51	Joback Method
dvisc	0.0005422	Pa×s	521.86	Joback Method
dvisc	0.0003940	Pa×s	570.22	Joback Method
dvisc	0.0003010	Pa×s	618.58	Joback Method
dvisc	0.0002391	Pa×s	666.93	Joback Method
dvisc	0.0001959	Pa×s	715.29	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2876746&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

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

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