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
CAS: 2876-73-5

Physical Properties

Property code	Value	Unit	Source
gf	76.19	kJ/mol	Joback Method
hf	-243.52	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.506		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
tb	738.17	K	Joback Method
tc	950.21	K	Joback Method
tf	436.42	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.16	J/mol×K	738.17	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
cpg	728.02	J/mol×K	950.21	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	0.0003617	Pa×s	587.29	Joback Method
dvisc	0.0005022	Pa×s	537.00	Joback Method
dvisc	0.0007463	Pa×s	486.71	Joback Method
dvisc	0.0012149	Pa×s	436.42	Joback Method

Sources

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=C2876735&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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