1-Naphthaleneacetic acid, undecyl ester

Inchi: InChI=1S/C23H32O2/c1-2-3-4-5-6-7-8-9-12-18-25-23(24)19-21-16-13-15-20-14-10-11-17
InchiKey: BTBUEVCCILMYJY-UHFFFAOYSA-N
Formula: C23H32O2
SMILES: CCCCCCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	118.29	kJ/mol	Joback Method
hf	-346.72	kJ/mol	Joback Method
hfus	48.78	kJ/mol	Joback Method
hvap	80.53	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.456		Crippen Method
mcvol	299.150	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	852.57	K	Joback Method
tc	1058.18	K	Joback Method
tf	492.77	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.53	J/mol×K	852.57	Joback Method
cpg	950.91	J/mol×K	886.84	Joback Method
cpg	967.21	J/mol×K	921.11	Joback Method
cpg	982.53	J/mol×K	955.37	Joback Method
cpg	996.91	J/mol×K	989.64	Joback Method
cpg	1010.44	J/mol×K	1023.91	Joback Method
cpg	1023.17	J/mol×K	1058.18	Joback Method
dvisc	0.0008576	Pa×s	492.77	Joback Method

dvisc	0.0004915	Pa×s	552.74	Joback Method
dvisc	0.0003141	Pa×s	612.70	Joback Method
dvisc	0.0002174	Pa×s	672.67	Joback Method
dvisc	0.0001598	Pa×s	732.64	Joback Method
dvisc	0.0001231	Pa×s	792.60	Joback Method
dvisc	0.0000983	Pa×s	852.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415034&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume