1-Naphthaleneacetic acid, tridecyl ester

Inchi: InChI=1S/C25H36O2/c1-2-3-4-5-6-7-8-9-10-11-14-20-27-25(26)21-23-18-15-17-22-16-12
InchiKey: CEXDNJXKGYFGNU-UHFFFAOYSA-N
Formula: C25H36O2
SMILES: CCCCCCCCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	135.13	kJ/mol	Joback Method
hf	-388.00	kJ/mol	Joback Method
hfus	53.96	kJ/mol	Joback Method
hvap	84.98	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	7.237		Crippen Method
mcvol	327.330	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	1844.00		NIST Webbook
rinpol	1844.00		NIST Webbook
tb	898.33	K	Joback Method
tc	1106.00	K	Joback Method
tf	515.31	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.81	J/mol×K	898.33	Joback Method
cpg	1072.68	J/mol×K	932.94	Joback Method
cpg	1089.46	J/mol×K	967.55	Joback Method
cpg	1105.23	J/mol×K	1002.16	Joback Method
cpg	1120.05	J/mol×K	1036.77	Joback Method
cpg	1134.01	J/mol×K	1071.38	Joback Method
cpg	1147.18	J/mol×K	1106.00	Joback Method
dvisc	0.0007179	Pa×s	515.31	Joback Method

dvisc	0.0004014	Pa×s	579.15	Joback Method
dvisc	0.0002519	Pa×s	642.98	Joback Method
dvisc	0.0001720	Pa×s	706.82	Joback Method
dvisc	0.0001251	Pa×s	770.66	Joback Method
dvisc	0.0000955	Pa×s	834.49	Joback Method
dvisc	0.0000758	Pa×s	898.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415036&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:
https://www.chemeo.com/cid/95-298-7/1-Naphthaleneacetic-acid-tridecyl-ester.pdf
Generated by Cheméo on 2024-10-12 06:11:53.613160077 +0000 UTC m=+3294376.250129325.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.