

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:	CCCCCCCCCCCCOC(=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004014	Paxs	579.15	Joback Method
dvisc	0.0002519	Paxs	642.98	Joback Method
dvisc	0.0001720	Paxs	706.82	Joback Method
dvisc	0.0001251	Paxs	770.66	Joback Method
dvisc	0.0000955	Paxs	834.49	Joback Method
dvisc	0.0000758	Paxs	898.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415036&Units=SI

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

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