1-Naphthaleneacetic acid, pentadecyl ester

Inchi: InChI=1S/C27H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-22-29-27(28)23-25-20-17-19-24
InchiKey: FZVAATALWMJBCF-UHFFFAOYSA-N
Formula: C27H40O2
SMILES: CCCCCCCCCCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 396.61

Physical Properties

Property code	Value	Unit	Source
gf	151.97	kJ/mol	Joback Method
hf	-429.28	kJ/mol	Joback Method
hfus	59.14	kJ/mol	Joback Method
hvap	89.43	kJ/mol	Joback Method
log10ws	-9.22		Crippen Method
logp	8.017		Crippen Method
mcvol	355.510	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	944.09	K	Joback Method
tc	1157.09	K	Joback Method
tf	537.85	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.82	J/mol×K	944.09	Joback Method
cpg	1197.33	J/mol×K	979.59	Joback Method
cpg	1214.71	J/mol×K	1015.09	Joback Method
cpg	1231.03	J/mol×K	1050.59	Joback Method
cpg	1246.39	J/mol×K	1086.09	Joback Method
cpg	1260.87	J/mol×K	1121.59	Joback Method
cpg	1274.57	J/mol×K	1157.09	Joback Method
dvisc	0.0005904	Pa×s	537.85	Joback Method

dvisc	0.0003227	Pa×s	605.56	Joback Method
dvisc	0.0001992	Pa×s	673.26	Joback Method
dvisc	0.0001343	Pa×s	740.97	Joback Method
dvisc	0.0000967	Pa×s	808.68	Joback Method
dvisc	0.0000733	Pa×s	876.38	Joback Method
dvisc	0.0000578	Pa×s	944.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415038&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