1-Naphthaleneacetic acid, hexadecyl ester

Inchi: InChI=1S/C28H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-23-30-28(29)24-26-21-18-20
InchiKey: DVPGWPZAZCGSIU-UHFFFAOYSA-N
Formula: C28H42O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	160.39	kJ/mol	Joback Method
hf	-449.92	kJ/mol	Joback Method
hfus	61.73	kJ/mol	Joback Method
hvap	91.66	kJ/mol	Joback Method
log10ws	-9.64		Crippen Method
logp	8.407		Crippen Method
mcvol	369.600	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinpol	2035.00		NIST Webbook
rinpol	2035.00		NIST Webbook
tb	966.97	K	Joback Method
tc	1184.01	K	Joback Method
tf	549.12	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1241.73	J/mol×K	966.97	Joback Method
cpg	1325.53	J/mol×K	1147.84	Joback Method
cpg	1310.73	J/mol×K	1111.67	Joback Method
cpg	1295.04	J/mol×K	1075.49	Joback Method
cpg	1278.38	J/mol×K	1039.32	Joback Method
cpg	1260.64	J/mol×K	1003.14	Joback Method
cpg	1339.54	J/mol×K	1184.01	Joback Method
dvisc	0.0000502	Pa×s	966.97	Joback Method

dvisc	0.0000639	Pa×s	897.33	Joback Method
dvisc	0.0000847	Pa×s	827.69	Joback Method
dvisc	0.0001181	Pa×s	758.05	Joback Method
dvisc	0.0001762	Pa×s	688.40	Joback Method
dvisc	0.0002878	Pa×s	618.76	Joback Method
dvisc	0.0005323	Pa×s	549.12	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=U415039&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume