9H-Fluorene-9-carboxylic acid, hexadecyl ester

Inchi: InChI=1S/C30H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-24-32-30(31)29-27-22-17-15

InchiKey: YQRZBRMWYAFGSW-UHFFFAOYSA-N

Formula: C30H42O2

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1c2ccccc2-c2ccccc21

Mol. weight [g/mol]: 434.65

Physical Properties

Property code	Value	Unit	Source
gf	258.31	kJ/mol	Joback Method
hf	-372.09	kJ/mol	Joback Method
hfus	65.88	kJ/mol	Joback Method
hvap	96.98	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	8.823		Crippen Method
mcvol	382.620	ml/mol	McGowan Method
pc	896.41	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	1023.61	K	Joback Method
tc	1253.22	K	Joback Method
tf	602.88	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.23	J/mol×K	1023.61	Joback Method
cpg	1410.59	J/mol×K	1214.95	Joback Method
cpg	1393.75	J/mol×K	1176.69	Joback Method
cpg	1376.44	J/mol×K	1138.42	Joback Method
cpg	1358.51	J/mol×K	1100.15	Joback Method
cpg	1339.83	J/mol×K	1061.88	Joback Method
cpg	1427.12	J/mol×K	1253.22	Joback Method
dvisc	0.0001481	Pa×s	1023.61	Joback Method

dvisc	0.0001776	Pa×s	953.49	Joback Method
dvisc	0.0002192	Pa×s	883.37	Joback Method
dvisc	0.0002804	Pa×s	813.25	Joback Method
dvisc	0.0003759	Pa×s	743.12	Joback Method
dvisc	0.0005356	Pa×s	673.00	Joback Method
dvisc	0.0008286	Pa×s	602.88	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=U415136&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