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

Inchi: InChI=1S/C31H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-25-33-31(32)30-28-23-18

InchiKey: LHNPJBDVFFQGID-UHFFFAOYSA-N

Formula: C31H44O2

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1c2ccccc2-c2ccccc21

Mol. weight [g/mol]: 448.68

Physical Properties

Property code	Value	Unit	Source
gf	266.73	kJ/mol	Joback Method
hf	-392.73	kJ/mol	Joback Method
hfus	68.47	kJ/mol	Joback Method
hvap	99.20	kJ/mol	Joback Method
log10ws	-10.78		Crippen Method
logp	9.213		Crippen Method
mcvol	396.710	ml/mol	McGowan Method
pc	847.02	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	1046.49	K	Joback Method
tc	1282.09	K	Joback Method
tf	614.15	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.64	J/mol×K	1046.49	Joback Method
cpg	1404.92	J/mol×K	1085.76	Joback Method
cpg	1424.30	J/mol×K	1125.02	Joback Method
cpg	1442.93	J/mol×K	1164.29	Joback Method
cpg	1460.99	J/mol×K	1203.55	Joback Method
cpg	1478.63	J/mol×K	1242.82	Joback Method
cpg	1496.01	J/mol×K	1282.09	Joback Method
dvisc	0.0007567	Pa×s	614.15	Joback Method

dvisc	0.0004835	Pa×s	686.21	Joback Method
dvisc	0.0003364	Pa×s	758.26	Joback Method
dvisc	0.0002493	Pa×s	830.32	Joback Method
dvisc	0.0001938	Pa×s	902.38	Joback Method
dvisc	0.0001563	Pa×s	974.43	Joback Method
dvisc	0.0001299	Pa×s	1046.49	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=U415137&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