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

Inchi: InChI=1S/C29H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-23-31-29(30)28-26-21-16-14-19

InchiKey: WTTDBZYCZYBRLW-UHFFFAOYSA-N

Formula: C29H40O2

SMILES: CCCCCCCCCCCCCCCOC(=O)C1c2ccccc2-c2ccccc21

Mol. weight [g/mol]: 420.63

Physical Properties

Property code	Value	Unit	Source
gf	249.89	kJ/mol	Joback Method
hf	-351.45	kJ/mol	Joback Method
hfus	63.29	kJ/mol	Joback Method
hvap	94.75	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.433		Crippen Method
mcvol	368.530	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	1000.73	K	Joback Method
tc	1225.47	K	Joback Method
tf	591.61	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.41	J/mol×K	1000.73	Joback Method
cpg	1275.41	J/mol×K	1038.19	Joback Method
cpg	1293.50	J/mol×K	1075.64	Joback Method
cpg	1310.81	J/mol×K	1113.10	Joback Method
cpg	1327.48	J/mol×K	1150.56	Joback Method
cpg	1343.65	J/mol×K	1188.01	Joback Method
cpg	1359.44	J/mol×K	1225.47	Joback Method
dvisc	0.0009038	Pa×s	591.61	Joback Method

dvisc	0.0005911	Pa×s	659.80	Joback Method
dvisc	0.0004185	Pa×s	727.98	Joback Method
dvisc	0.0003144	Pa×s	796.17	Joback Method
dvisc	0.0002471	Pa×s	864.36	Joback Method
dvisc	0.0002012	Pa×s	932.54	Joback Method
dvisc	0.0001684	Pa×s	1000.73	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=U415135&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