Fumaric acid, 3-hexyl nonadecyl ester

Inchi: InChI=1S/C29H54O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-26-32-28(30)25-27(31)33-29(24-6-3)23-5-2/h25,29H,4-24H2,1-3H3/b27-25+

InchiKey: WOAZNNHTWIHWQZ-OCOZRVBESA-N

Formula: C29H54O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCC

Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-196.76	kJ/mol	Joback Method
hf	-1019.55	kJ/mol	Joback Method
hfus	73.12	kJ/mol	Joback Method
hvap	98.03	kJ/mol	Joback Method
log10ws	-9.65		Crippen Method
logp	8.859		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	674.65	kPa	Joback Method
rinpol	3189.00		NIST Webbook
rinpol	3189.00		NIST Webbook
tb	1019.22	K	Joback Method
tc	1266.06	K	Joback Method
tf	540.83	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.74	J/mol×K	1019.22	Joback Method
cpg	1534.40	J/mol×K	1060.36	Joback Method
cpg	1555.11	J/mol×K	1101.50	Joback Method
cpg	1573.97	J/mol×K	1142.64	Joback Method
cpg	1591.09	J/mol×K	1183.78	Joback Method
cpg	1606.58	J/mol×K	1224.92	Joback Method
cpg	1620.54	J/mol×K	1266.06	Joback Method
dvisc	0.0002886	Pa×s	540.83	Joback Method

dvisc	0.0001173	Pa×s	620.56	Joback Method
dvisc	0.0000585	Pa×s	700.29	Joback Method
dvisc	0.0000336	Pa×s	780.02	Joback Method
dvisc	0.0000214	Pa×s	859.76	Joback Method
dvisc	0.0000147	Pa×s	939.49	Joback Method
dvisc	0.0000107	Pa×s	1019.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348617&Units=SI
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

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