Fumaric acid, 2-decyl octadecyl ester

Inchi: InChI=1S/C32H60O4/c1-4-6-8-10-12-13-14-15-16-17-18-19-20-21-23-25-29-35-31(33)27
InchiKey: QOSRDEQJEKDXHQ-BYYHNAKLSA-N
Formula: C32H60O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCCCCCC
Mol. weight [g/mol]: 508.82

Physical Properties

Property code	Value	Unit	Source
gf	-171.50	kJ/mol	Joback Method
hf	-1081.47	kJ/mol	Joback Method
hfus	80.89	kJ/mol	Joback Method
hvap	104.71	kJ/mol	Joback Method
log10ws	-10.91		Crippen Method
logp	10.030		Crippen Method
mcvol	472.320	ml/mol	McGowan Method
pc	584.01	kPa	Joback Method
rinpol	3490.00		NIST Webbook
rinpol	3490.00		NIST Webbook
tb	1087.86	K	Joback Method
tc	1377.88	K	Joback Method
tf	574.64	K	Joback Method
vc	1.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1708.59	J/mol×K	1087.86	Joback Method
cpg	1810.95	J/mol×K	1329.55	Joback Method
cpg	1794.93	J/mol×K	1281.21	Joback Method
cpg	1776.88	J/mol×K	1232.87	Joback Method
cpg	1756.60	J/mol×K	1184.53	Joback Method
cpg	1733.90	J/mol×K	1136.20	Joback Method
cpg	1825.13	J/mol×K	1377.88	Joback Method
dvisc	0.0000066	Pa×s	1087.86	Joback Method

dvisc	0.0000091	Pa×s	1002.32	Joback Method
dvisc	0.0000133	Pa×s	916.79	Joback Method
dvisc	0.0000210	Pa×s	831.25	Joback Method
dvisc	0.0000369	Pa×s	745.71	Joback Method
dvisc	0.0000748	Pa×s	660.18	Joback Method
dvisc	0.0001875	Pa×s	574.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348599&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