Fumaric acid, 2-decyl nonadecyl ester

Inchi: InChI=1S/C33H62O4/c1-4-6-8-10-12-13-14-15-16-17-18-19-20-21-22-24-26-30-36-32(34
InchiKey: DCRUNYSYJXFGGA-ZQHSETAFSA-N
Formula: C33H62O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCCCCCC
Mol. weight [g/mol]: 522.84

Physical Properties

Property code	Value	Unit	Source
gf	-163.08	kJ/mol	Joback Method
hf	-1102.11	kJ/mol	Joback Method
hfus	83.48	kJ/mol	Joback Method
hvap	106.93	kJ/mol	Joback Method
log10ws	-11.33		Crippen Method
logp	10.420		Crippen Method
mcvol	486.410	ml/mol	McGowan Method
pc	557.83	kPa	Joback Method
rinpol	3606.00		NIST Webbook
rinpol	3606.00		NIST Webbook
tb	1110.74	K	Joback Method
tc	1418.73	K	Joback Method
tf	585.91	K	Joback Method
vc	1.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1774.71	J/mol×K	1110.74	Joback Method
cpg	1801.07	J/mol×K	1162.07	Joback Method
cpg	1824.52	J/mol×K	1213.40	Joback Method
cpg	1845.31	J/mol×K	1264.73	Joback Method
cpg	1863.69	J/mol×K	1316.06	Joback Method
cpg	1879.90	J/mol×K	1367.40	Joback Method
cpg	1894.19	J/mol×K	1418.73	Joback Method
dvisc	0.0001618	Pa×s	585.91	Joback Method

dvisc	0.0000642	Pa×s	673.38	Joback Method
dvisc	0.0000315	Pa×s	760.85	Joback Method
dvisc	0.0000179	Pa×s	848.33	Joback Method
dvisc	0.0000113	Pa×s	935.80	Joback Method
dvisc	0.0000077	Pa×s	1023.27	Joback Method
dvisc	0.0000056	Pa×s	1110.74	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=U348600&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