Fumaric acid, 2-methylpent-3-yl nonadecyl ester

Inchi: InChI=1S/C29H54O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-32-28(30)
InchiKey: JCFTYYFBNKVCRN-WCWDXBQESA-N
Formula: C29H54O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-199.20	kJ/mol	Joback Method
hf	-1024.83	kJ/mol	Joback Method
hfus	69.60	kJ/mol	Joback Method
hvap	97.64	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	8.715		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	677.46	kPa	Joback Method
rinpol	3171.00		NIST Webbook
tb	1018.78	K	Joback Method
tc	1263.11	K	Joback Method
tf	525.83	K	Joback Method
vc	1.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.99	J/mol×K	1018.78	Joback Method
cpg	1534.35	J/mol×K	1059.50	Joback Method
cpg	1554.79	J/mol×K	1100.22	Joback Method
cpg	1573.39	J/mol×K	1140.94	Joback Method
cpg	1590.27	J/mol×K	1181.67	Joback Method
cpg	1605.53	J/mol×K	1222.39	Joback Method
cpg	1619.27	J/mol×K	1263.11	Joback Method
dvisc	0.0003313	Pa×s	525.83	Joback Method
dvisc	0.0001238	Pa×s	607.99	Joback Method

dvisc	0.0000585	Pa×s	690.15	Joback Method
dvisc	0.0000324	Pa×s	772.31	Joback Method
dvisc	0.0000201	Pa×s	854.46	Joback Method
dvisc	0.0000136	Pa×s	936.62	Joback Method
dvisc	0.0000098	Pa×s	1018.78	Joback Method

Sources

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=U348775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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