Fumaric acid, tetradec-3-enyl undecyl ester

Inchi: InChI=1S/C29H52O4/c1-3-5-7-9-11-13-14-15-17-19-21-23-27-33-29(31)25-24-28(30)32-
InchiKey: NZABBEYBGSAODK-UBSPVRHQSA-N
Formula: C29H52O4
SMILES: CCCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-114.10	kJ/mol	Joback Method
hf	-897.05	kJ/mol	Joback Method
hfus	76.84	kJ/mol	Joback Method
hvap	98.38	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.637		Crippen Method
mcvol	425.750	ml/mol	McGowan Method
pc	690.34	kPa	Joback Method
rinpol	3304.00		NIST Webbook
tb	1023.82	K	Joback Method
tc	1270.20	K	Joback Method
tf	550.75	K	Joback Method
vc	1.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1483.21	J/mol×K	1023.82	Joback Method
cpg	1505.71	J/mol×K	1064.88	Joback Method
cpg	1526.52	J/mol×K	1105.95	Joback Method
cpg	1545.76	J/mol×K	1147.01	Joback Method
cpg	1563.57	J/mol×K	1188.07	Joback Method
cpg	1580.07	J/mol×K	1229.14	Joback Method
cpg	1595.38	J/mol×K	1270.20	Joback Method
dvisc	0.0002376	Pa×s	550.75	Joback Method
dvisc	0.0001018	Pa×s	629.60	Joback Method

dvisc	0.0000526	Pa×s	708.44	Joback Method
dvisc	0.0000311	Pa×s	787.29	Joback Method
dvisc	0.0000202	Pa×s	866.13	Joback Method
dvisc	0.0000141	Pa×s	944.98	Joback Method
dvisc	0.0000104	Pa×s	1023.82	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=U348842&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