Fumaric acid, eicosyl trans-hex-3-enyl ester

Inchi: InChI=1S/C30H54O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-28-34-30(
InchiKey: AQVUQOMWTPNHRB-XZCLYGNBSA-N
Formula: C30H54O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-105.68	kJ/mol	Joback Method
hf	-917.69	kJ/mol	Joback Method
hfus	79.43	kJ/mol	Joback Method
hvap	100.60	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	9.027		Crippen Method
mcvol	439.840	ml/mol	McGowan Method
pc	656.79	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1046.70	K	Joback Method
tc	1305.52	K	Joback Method
tf	562.02	K	Joback Method
vc	1.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.54	J/mol×K	1046.70	Joback Method
cpg	1571.96	J/mol×K	1089.84	Joback Method
cpg	1593.55	J/mol×K	1132.97	Joback Method
cpg	1613.46	J/mol×K	1176.11	Joback Method
cpg	1631.83	J/mol×K	1219.25	Joback Method
cpg	1648.81	J/mol×K	1262.38	Joback Method
cpg	1664.56	J/mol×K	1305.52	Joback Method
dvisc	0.0002071	Pa×s	562.02	Joback Method

dvisc	0.0000881	Pa×s	642.80	Joback Method
dvisc	0.0000453	Pa×s	723.58	Joback Method
dvisc	0.0000267	Pa×s	804.36	Joback Method
dvisc	0.0000173	Pa×s	885.14	Joback Method
dvisc	0.0000120	Pa×s	965.92	Joback Method
dvisc	0.0000089	Pa×s	1046.70	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348899&Units=SI

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