Fumaric acid, octyl tetradec-3-enyl ester

Inchi: InChI=1S/C26H46O4/c1-3-5-7-9-11-12-13-14-15-16-18-20-24-30-26(28)22-21-25(27)29-
InchiKey: OGGGKARWIPVHJJ-HLSPWXCOSA-N
Formula: C26H46O4
SMILES: CCCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCCCCCC
Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-139.36	kJ/mol	Joback Method
hf	-835.13	kJ/mol	Joback Method
hfus	69.07	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.467		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinpol	2998.00		NIST Webbook
rinpol	2998.00		NIST Webbook
tb	955.18	K	Joback Method
tc	1172.59	K	Joback Method
tf	516.94	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.79	J/mol×K	955.18	Joback Method
cpg	1309.98	J/mol×K	991.42	Joback Method
cpg	1328.84	J/mol×K	1027.65	Joback Method
cpg	1346.43	J/mol×K	1063.89	Joback Method
cpg	1362.84	J/mol×K	1100.12	Joback Method
cpg	1378.13	J/mol×K	1136.36	Joback Method
cpg	1392.39	J/mol×K	1172.59	Joback Method
dvisc	0.0003540	Pa×s	516.94	Joback Method

dvisc	0.0001550	Pa×s	589.98	Joback Method
dvisc	0.0000814	Pa×s	663.02	Joback Method
dvisc	0.0000486	Pa×s	736.06	Joback Method
dvisc	0.0000319	Pa×s	809.10	Joback Method
dvisc	0.0000224	Pa×s	882.14	Joback Method
dvisc	0.0000166	Pa×s	955.18	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=U348839&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