Fumaric acid, cis-hex-3-enyl nonyl ester

Inchi: InChI=1S/C19H32O4/c1-3-5-7-9-10-11-13-17-23-19(21)15-14-18(20)22-16-12-8-6-4-2/h6
InchiKey: NJWASWXUKVCZRT-GNYNHFTISA-N
Formula: C19H32O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-198.30	kJ/mol	Joback Method
hf	-690.65	kJ/mol	Joback Method
hfus	50.94	kJ/mol	Joback Method
hvap	76.12	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.736		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook
tb	795.02	K	Joback Method
tc	982.06	K	Joback Method
tf	438.05	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.06	J/mol×K	795.02	Joback Method
cpg	934.02	J/mol×K	950.88	Joback Method
cpg	920.71	J/mol×K	919.71	Joback Method
cpg	906.59	J/mol×K	888.54	Joback Method
cpg	891.63	J/mol×K	857.37	Joback Method
cpg	875.80	J/mol×K	826.19	Joback Method
cpg	946.55	J/mol×K	982.06	Joback Method
dvisc	0.0000463	Pa×s	795.02	Joback Method

dvisc	0.0000616	Pa×s	735.52	Joback Method
dvisc	0.0000859	Pa×s	676.03	Joback Method
dvisc	0.0001279	Pa×s	616.53	Joback Method
dvisc	0.0002074	Pa×s	557.04	Joback Method
dvisc	0.0003774	Pa×s	497.55	Joback Method
dvisc	0.0008079	Pa×s	438.05	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=U348865&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