Fumaric acid, di(cis-non-3-enyl) ester

Inchi: InChI=1S/C22H36O4/c1-3-5-7-9-11-13-15-19-25-21(23)17-18-22(24)26-20-16-14-12-10-
InchiKey: ZYZUJFGICIVOFR-VKHQDECPSA-N
Formula: C22H36O4
SMILES: CCCCCC=CCCOC(=O)C=CC(=O)OCCC=CCCCCC
Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-92.82	kJ/mol	Joback Method
hf	-635.35	kJ/mol	Joback Method
hfus	58.92	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.682		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2581.00		NIST Webbook
tb	867.82	K	Joback Method
tc	1064.59	K	Joback Method
tf	466.78	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.82	J/mol×K	867.82	Joback Method
cpg	1030.30	J/mol×K	900.62	Joback Method
cpg	1046.82	J/mol×K	933.41	Joback Method
cpg	1062.43	J/mol×K	966.21	Joback Method
cpg	1077.19	J/mol×K	999.00	Joback Method
cpg	1091.15	J/mol×K	1031.80	Joback Method
cpg	1104.37	J/mol×K	1064.59	Joback Method
dvisc	0.0005393	Pa×s	466.78	Joback Method
dvisc	0.0002381	Pa×s	533.62	Joback Method

dvisc	0.0001261	Pa×s	600.46	Joback Method
dvisc	0.0000758	Pa×s	667.30	Joback Method
dvisc	0.0000500	Pa×s	734.14	Joback Method
dvisc	0.0000354	Pa×s	800.98	Joback Method
dvisc	0.0000264	Pa×s	867.82	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=U348882&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