Fumaric acid, butyl tetradec-3-enyl ester

Inchi: InChI=1S/C22H38O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-20-26-22(24)18-17-21(23)25-1
InchiKey: YJGNPNFLMOVAME-QYWXAPKASA-N
Formula: C22H38O4
SMILES: CCCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-173.04	kJ/mol	Joback Method
hf	-752.57	kJ/mol	Joback Method
hfus	58.71	kJ/mol	Joback Method
hvap	82.79	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.906		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	2597.00		NIST Webbook
rinpol	2597.00		NIST Webbook
tb	863.66	K	Joback Method
tc	1058.41	K	Joback Method
tf	471.86	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.41	J/mol×K	863.66	Joback Method
cpg	1119.40	J/mol×K	1025.96	Joback Method
cpg	1105.31	J/mol×K	993.50	Joback Method
cpg	1090.31	J/mol×K	961.04	Joback Method
cpg	1074.36	J/mol×K	928.58	Joback Method
cpg	1057.40	J/mol×K	896.12	Joback Method
cpg	1132.62	J/mol×K	1058.41	Joback Method
dvisc	0.0000302	Pa×s	863.66	Joback Method

dvisc	0.0000405	Pa×s	798.36	Joback Method
dvisc	0.0000570	Pa×s	733.06	Joback Method
dvisc	0.0000858	Pa×s	667.76	Joback Method
dvisc	0.0001413	Pa×s	602.46	Joback Method
dvisc	0.0002626	Pa×s	537.16	Joback Method
dvisc	0.0005794	Pa×s	471.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348517&Units=SI
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

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