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

Inchi: InChI=1S/C21H36O4/c1-3-5-7-9-10-11-12-13-15-19-25-21(23)17-16-20(22)24-18-14-8-6
InchiKey: NIZVQRSQQBISTA-JNKFDQBJSA-N
Formula: C21H36O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-181.46	kJ/mol	Joback Method
hf	-731.93	kJ/mol	Joback Method
hfus	56.12	kJ/mol	Joback Method
hvap	80.57	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.516		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2475.00		NIST Webbook
tb	840.78	K	Joback Method
tc	1032.19	K	Joback Method
tf	460.59	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.48	J/mol×K	840.78	Joback Method
cpg	996.04	J/mol×K	872.68	Joback Method
cpg	1012.60	J/mol×K	904.58	Joback Method
cpg	1028.21	J/mol×K	936.48	Joback Method
cpg	1042.91	J/mol×K	968.39	Joback Method
cpg	1056.73	J/mol×K	1000.29	Joback Method
cpg	1069.73	J/mol×K	1032.19	Joback Method
dvisc	0.0006498	Pa×s	460.59	Joback Method
dvisc	0.0002974	Pa×s	523.96	Joback Method

dvisc	0.0001611	Pa×s	587.32	Joback Method
dvisc	0.0000984	Pa×s	650.69	Joback Method
dvisc	0.0000655	Pa×s	714.05	Joback Method
dvisc	0.0000467	Pa×s	777.42	Joback Method
dvisc	0.0000350	Pa×s	840.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348891&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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