Fumaric acid, pent-4-enyl tridecyl ester

Inchi: InChI=1S/C22H38O4/c1-3-5-7-8-9-10-11-12-13-14-16-20-26-22(24)18-17-21(23)25-19-1
InchiKey: UTUKZCICGXSHOA-ISLYRVAYSA-N
Formula: C22H38O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-165.42	kJ/mol	Joback Method
hf	-744.36	kJ/mol	Joback Method
hfus	57.23	kJ/mol	Joback Method
hvap	82.17	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.906		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2583.00		NIST Webbook
rinpol	2583.00		NIST Webbook
tb	856.18	K	Joback Method
tc	1049.03	K	Joback Method
tf	475.18	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.85	J/mol×K	856.18	Joback Method
cpg	1117.47	J/mol×K	1016.89	Joback Method
cpg	1103.55	J/mol×K	984.74	Joback Method
cpg	1088.66	J/mol×K	952.60	Joback Method
cpg	1072.77	J/mol×K	920.46	Joback Method
cpg	1055.85	J/mol×K	888.32	Joback Method
cpg	1130.47	J/mol×K	1049.03	Joback Method
dvisc	0.0000372	Pa×s	856.18	Joback Method

dvisc	0.0000493	Pa×s	792.68	Joback Method
dvisc	0.0000688	Pa×s	729.18	Joback Method
dvisc	0.0001023	Pa×s	665.68	Joback Method
dvisc	0.0001653	Pa×s	602.18	Joback Method
dvisc	0.0002991	Pa×s	538.68	Joback Method
dvisc	0.0006342	Pa×s	475.18	Joback Method

Sources

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=U348853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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