Fumaric acid, pentyl tridecyl ester

Inchi: InChI=1S/C22H40O4/c1-3-5-7-8-9-10-11-12-13-14-16-20-26-22(24)18-17-21(23)25-19-15-6-4-2
InchiKey: PLBGBCRZNSXECB-ISLYRVAYSA-N
Formula: C22H40O4
SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-253.26	kJ/mol	Joback Method
hf	-869.79	kJ/mol	Joback Method
hfus	58.51	kJ/mol	Joback Method
hvap	82.84	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	985.16	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	859.50	K	Joback Method
tc	1052.62	K	Joback Method
tf	476.94	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.82	J/mol×K	859.50	Joback Method
cpg	1147.73	J/mol×K	1020.43	Joback Method
cpg	1133.46	J/mol×K	988.25	Joback Method
cpg	1118.16	J/mol×K	956.06	Joback Method
cpg	1101.82	J/mol×K	923.87	Joback Method
cpg	1084.38	J/mol×K	891.69	Joback Method
cpg	1161.02	J/mol×K	1052.62	Joback Method
dvisc	0.0000347	Pa×s	859.50	Joback Method

dvisc	0.0000463	Pa×s	795.74	Joback Method
dvisc	0.0000649	Pa×s	731.98	Joback Method
dvisc	0.0000972	Pa×s	668.22	Joback Method
dvisc	0.0001584	Pa×s	604.46	Joback Method
dvisc	0.0002897	Pa×s	540.70	Joback Method
dvisc	0.0006226	Pa×s	476.94	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=U348805&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