Fumaric acid, dodecyl pent-4-enyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-173.84	kJ/mol	Joback Method
hf	-723.72	kJ/mol	Joback Method
hfus	54.64	kJ/mol	Joback Method
hvap	79.94	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.516		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	833.30	K	Joback Method
tc	1022.64	K	Joback Method
tf	463.91	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.99	J/mol×K	833.30	Joback Method
cpg	994.55	J/mol×K	864.86	Joback Method
cpg	1011.10	J/mol×K	896.41	Joback Method
cpg	1026.66	J/mol×K	927.97	Joback Method
cpg	1041.28	J/mol×K	959.53	Joback Method
cpg	1054.97	J/mol×K	991.08	Joback Method
cpg	1067.79	J/mol×K	1022.64	Joback Method
dvisc	0.0007093	Pa×s	463.91	Joback Method

dvisc	0.0003379	Pa×s	525.48	Joback Method
dvisc	0.0001881	Pa×s	587.04	Joback Method
dvisc	0.0001170	Pa×s	648.61	Joback Method
dvisc	0.0000790	Pa×s	710.17	Joback Method
dvisc	0.0000568	Pa×s	771.74	Joback Method
dvisc	0.0000429	Pa×s	833.30	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=U348852&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