Fumaric acid, 2-pentyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C21H36O4/c1-4-6-7-8-9-10-11-12-13-14-18-24-20(22)16-17-21(23)25-19(3)15
InchiKey: WNTLQWODZAODBM-VLDVYECUSA-N
Formula: C21H36O4
SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)OC(C)CCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-183.90	kJ/mol	Joback Method
hf	-737.21	kJ/mol	Joback Method
hfus	52.60	kJ/mol	Joback Method
hvap	80.18	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.514		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	2408.00		NIST Webbook
rinpol	2408.00		NIST Webbook
tb	840.34	K	Joback Method
tc	1032.59	K	Joback Method
tf	445.59	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.97	J/mol×K	840.34	Joback Method
cpg	1057.38	J/mol×K	1000.55	Joback Method
cpg	1043.56	J/mol×K	968.51	Joback Method
cpg	1028.85	J/mol×K	936.47	Joback Method
cpg	1013.21	J/mol×K	904.42	Joback Method
cpg	996.60	J/mol×K	872.38	Joback Method
cpg	1070.35	J/mol×K	1032.59	Joback Method
dvisc	0.0000320	Pa×s	840.34	Joback Method

dvisc	0.0000435	Pa×s	774.55	Joback Method
dvisc	0.0000624	Pa×s	708.76	Joback Method
dvisc	0.0000964	Pa×s	642.96	Joback Method
dvisc	0.0001645	Pa×s	577.17	Joback Method
dvisc	0.0003221	Pa×s	511.38	Joback Method
dvisc	0.0007690	Pa×s	445.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405566&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