Fumaric acid, 3-phenylpropyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C25H36O4/c1-2-3-4-5-6-7-8-9-10-14-21-28-24(26)19-20-25(27)29-22-15-18-23

InchiKey: MHYIYWBULBBIGN-PVLGCOFDSA-N

Formula: C25H36O4

SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-35.37	kJ/mol	Joback Method
hf	-577.96	kJ/mol	Joback Method
hfus	60.52	kJ/mol	Joback Method
hvap	91.75	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.959		Crippen Method
mcvol	345.630	ml/mol	McGowan Method
pc	1046.65	kPa	Joback Method
rinpol	3016.00		NIST Webbook
rinpol	3016.00		NIST Webbook
tb	958.98	K	Joback Method
tc	1174.97	K	Joback Method
tf	532.09	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.52	J/mol×K	958.98	Joback Method
cpg	1142.22	J/mol×K	994.98	Joback Method
cpg	1157.76	J/mol×K	1030.98	Joback Method
cpg	1172.24	J/mol×K	1066.97	Joback Method
cpg	1185.73	J/mol×K	1102.97	Joback Method
cpg	1198.30	J/mol×K	1138.97	Joback Method
cpg	1210.04	J/mol×K	1174.97	Joback Method
dvisc	0.0003392	Pa×s	532.09	Joback Method

dvisc	0.0001601	Pa×s	603.24	Joback Method
dvisc	0.0000885	Pa×s	674.39	Joback Method
dvisc	0.0000548	Pa×s	745.54	Joback Method
dvisc	0.0000369	Pa×s	816.68	Joback Method
dvisc	0.0000265	Pa×s	887.83	Joback Method
dvisc	0.0000199	Pa×s	958.98	Joback Method

Sources

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=U405672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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