Fumaric acid, 3,5-dimethylphenyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C24H34O4/c1-4-5-6-7-8-9-10-11-12-13-16-27-23(25)14-15-24(26)28-22-18-20

InchiKey: AEFAUOCCFJSWSU-SQIWNDBBSA-N

Formula: C24H34O4

SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 386.52

Physical Properties

Property code	Value	Unit	Source
gf	-63.05	kJ/mol	Joback Method
hf	-580.26	kJ/mol	Joback Method
hfus	57.16	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.005		Crippen Method
mcvol	331.540	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	946.06	K	Joback Method
tc	1160.68	K	Joback Method
tf	545.86	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.77	J/mol×K	946.06	Joback Method
cpg	1078.98	J/mol×K	981.83	Joback Method
cpg	1094.05	J/mol×K	1017.60	Joback Method
cpg	1108.04	J/mol×K	1053.37	Joback Method
cpg	1121.00	J/mol×K	1089.14	Joback Method
cpg	1132.99	J/mol×K	1124.91	Joback Method
cpg	1144.08	J/mol×K	1160.68	Joback Method
dvisc	0.0002863	Pa×s	545.86	Joback Method

dvisc	0.0001515	Pa×s	612.56	Joback Method
dvisc	0.0000909	Pa×s	679.26	Joback Method
dvisc	0.0000597	Pa×s	745.96	Joback Method
dvisc	0.0000420	Pa×s	812.66	Joback Method
dvisc	0.0000312	Pa×s	879.36	Joback Method
dvisc	0.0000242	Pa×s	946.06	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=U405746&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