Fumaric acid, 2,4,4-trimethylpentyl dec-2-yl ester

Inchi: InChI=1S/C22H40O4/c1-7-8-9-10-11-12-13-19(3)26-21(24)15-14-20(23)25-17-18(2)16-2

InchiKey: QEQSFFFLNFKJIU-CCEZHUSRSA-N

Formula: C22H40O4

SMILES: CCCCCCCCC(C)OC(=O)C=CC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-255.30	kJ/mol	Joback Method
hf	-889.10	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	80.76	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.840		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	855.39	K	Joback Method
tc	1050.84	K	Joback Method
tf	449.36	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.29	J/mol×K	855.39	Joback Method
cpg	1085.84	J/mol×K	887.96	Joback Method
cpg	1103.27	J/mol×K	920.54	Joback Method
cpg	1119.61	J/mol×K	953.11	Joback Method
cpg	1134.92	J/mol×K	985.69	Joback Method
cpg	1149.24	J/mol×K	1018.26	Joback Method
cpg	1162.64	J/mol×K	1050.84	Joback Method
dvisc	0.0008403	Pa×s	449.36	Joback Method

dvisc	0.0003111	Pa×s	517.03	Joback Method
dvisc	0.0001450	Pa×s	584.70	Joback Method
dvisc	0.0000792	Pa×s	652.38	Joback Method
dvisc	0.0000484	Pa×s	720.05	Joback Method
dvisc	0.0000322	Pa×s	787.72	Joback Method
dvisc	0.0000229	Pa×s	855.39	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=U405610&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