Fumaric acid, 2,4-dimethylpent-3-yl undecyl ester

Inchi: InChI=1S/C22H40O4/c1-6-7-8-9-10-11-12-13-14-17-25-20(23)15-16-21(24)26-22(18(2)3

InchiKey: NLQHFNWCOXBYBB-FOCLMDBBSA-N

Formula: C22H40O4

SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-260.58	kJ/mol	Joback Method
hf	-885.63	kJ/mol	Joback Method
hfus	47.94	kJ/mol	Joback Method
hvap	81.67	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.840		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	858.18	K	Joback Method
tc	1052.55	K	Joback Method
tf	431.94	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.21	J/mol×K	858.18	Joback Method
cpg	1149.10	J/mol×K	1020.16	Joback Method
cpg	1134.92	J/mol×K	987.76	Joback Method
cpg	1119.68	J/mol×K	955.37	Joback Method
cpg	1103.33	J/mol×K	922.97	Joback Method
cpg	1085.86	J/mol×K	890.58	Joback Method
cpg	1162.25	J/mol×K	1052.55	Joback Method
dvisc	0.0000266	Pa×s	858.18	Joback Method

dvisc	0.0000373	Pa×s	787.14	Joback Method
dvisc	0.0000559	Pa×s	716.10	Joback Method
dvisc	0.0000915	Pa×s	645.06	Joback Method
dvisc	0.0001694	Pa×s	574.02	Joback Method
dvisc	0.0003730	Pa×s	502.98	Joback Method
dvisc	0.0010648	Pa×s	431.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348552&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