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

Inchi: InChI=1S/C25H46O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-20-28-23(26)18-19-24(27)29-

InchiKey: IANLJONKIANLAJ-VHEBQXMUSA-N

Formula: C25H46O4

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

Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-235.32	kJ/mol	Joback Method
hf	-947.55	kJ/mol	Joback Method
hfus	55.71	kJ/mol	Joback Method
hvap	88.35	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	7.011		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
rinpol	2720.00		NIST Webbook
tb	926.82	K	Joback Method
tc	1135.15	K	Joback Method
tf	465.75	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.98	J/mol×K	926.82	Joback Method
cpg	1274.83	J/mol×K	961.54	Joback Method
cpg	1293.27	J/mol×K	996.26	Joback Method
cpg	1310.37	J/mol×K	1030.99	Joback Method
cpg	1326.17	J/mol×K	1065.71	Joback Method
cpg	1340.72	J/mol×K	1100.43	Joback Method
cpg	1354.08	J/mol×K	1135.15	Joback Method
dvisc	0.0006986	Pa×s	465.75	Joback Method
dvisc	0.0002417	Pa×s	542.60	Joback Method

dvisc	0.0001088	Pa×s	619.44	Joback Method
dvisc	0.0000584	Pa×s	696.29	Joback Method
dvisc	0.0000355	Pa×s	773.13	Joback Method
dvisc	0.0000236	Pa×s	849.98	Joback Method
dvisc	0.0000168	Pa×s	926.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348555&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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