Fumaric acid, 3,3-dimethylbut-2-yl tetradecyl ester

Inchi: InChI=1S/C24H44O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-20-27-22(25)18-19-23(26)28-
InchiKey: FIPKYXYUVVUDBT-VHEBQXMUSA-N
Formula: C24H44O4
SMILES: CCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-236.02	kJ/mol	Joback Method
hf	-925.10	kJ/mol	Joback Method
hfus	52.76	kJ/mol	Joback Method
hvap	85.60	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.765		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	890.54	kPa	Joback Method
rinpol	2642.00		NIST Webbook
tb	901.59	K	Joback Method
tc	1103.88	K	Joback Method
tf	486.90	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.07	J/mol×K	901.59	Joback Method
cpg	1210.34	J/mol×K	935.31	Joback Method
cpg	1228.40	J/mol×K	969.02	Joback Method
cpg	1245.30	J/mol×K	1002.74	Joback Method
cpg	1261.11	J/mol×K	1036.45	Joback Method
cpg	1275.87	J/mol×K	1070.17	Joback Method
cpg	1289.67	J/mol×K	1103.88	Joback Method
dvisc	0.0005269	Pa×s	486.90	Joback Method
dvisc	0.0002122	Pa×s	556.01	Joback Method

dvisc	0.0001045	Pa×s	625.13	Joback Method
dvisc	0.0000593	Pa×s	694.25	Joback Method
dvisc	0.0000373	Pa×s	763.36	Joback Method
dvisc	0.0000253	Pa×s	832.48	Joback Method
dvisc	0.0000182	Pa×s	901.59	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U348713&Units=SI

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