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

Inchi: InChI=1S/C26H48O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-21-29-24(27)19-20-25(28)
InchiKey: GAPFCPGZMUJRFZ-FMQUCBEESA-N
Formula: C26H48O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-226.90	kJ/mol	Joback Method
hf	-968.19	kJ/mol	Joback Method
hfus	58.30	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	7.401		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	2860.00		NIST Webbook
tb	949.70	K	Joback Method
tc	1164.67	K	Joback Method
tf	477.02	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.66	J/mol×K	949.70	Joback Method
cpg	1338.98	J/mol×K	985.53	Joback Method
cpg	1357.81	J/mol×K	1021.36	Joback Method
cpg	1375.19	J/mol×K	1057.19	Joback Method
cpg	1391.19	J/mol×K	1093.01	Joback Method
cpg	1405.87	J/mol×K	1128.84	Joback Method
cpg	1419.28	J/mol×K	1164.67	Joback Method
dvisc	0.0006042	Pa×s	477.02	Joback Method
dvisc	0.0002082	Pa×s	555.80	Joback Method

dvisc	0.0000935	Pa×s	634.58	Joback Method
dvisc	0.0000501	Pa×s	713.36	Joback Method
dvisc	0.0000304	Pa×s	792.14	Joback Method
dvisc	0.0000202	Pa×s	870.92	Joback Method
dvisc	0.0000143	Pa×s	949.70	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=U348556&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