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

Inchi: InChI=1S/C27H50O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-30-25(28)20-21-26(

InchiKey: XWMIVKGQPOVIOP-QZQOTICOSA-N

Formula: C27H50O4

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

Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-218.48	kJ/mol	Joback Method
hf	-988.83	kJ/mol	Joback Method
hfus	60.89	kJ/mol	Joback Method
hvap	92.80	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	7.791		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	753.91	kPa	Joback Method
rinpol	2936.00		NIST Webbook
rinpol	2936.00		NIST Webbook
tb	972.58	K	Joback Method
tc	1195.32	K	Joback Method
tf	488.29	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.79	J/mol×K	972.58	Joback Method
cpg	1471.58	J/mol×K	1158.19	Joback Method
cpg	1456.78	J/mol×K	1121.07	Joback Method
cpg	1440.57	J/mol×K	1083.95	Joback Method
cpg	1422.88	J/mol×K	1046.83	Joback Method
cpg	1403.65	J/mol×K	1009.70	Joback Method
cpg	1485.05	J/mol×K	1195.32	Joback Method
dvisc	0.0000122	Pa×s	972.58	Joback Method

dvisc	0.0000172	Pa×s	891.87	Joback Method
dvisc	0.0000260	Pa×s	811.15	Joback Method
dvisc	0.0000429	Pa×s	730.43	Joback Method
dvisc	0.0000802	Pa×s	649.72	Joback Method
dvisc	0.0001791	Pa×s	569.00	Joback Method
dvisc	0.0005216	Pa×s	488.29	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=U348557&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

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