Fumaric acid, 3-methylbut-2-yl octadecyl ester

Inchi: InChI=1S/C27H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-30-26(28)21-2
InchiKey: ZFDMIYUQICYKLT-QURGRASLSA-N
Formula: C27H50O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-216.04	kJ/mol	Joback Method
hf	-983.55	kJ/mol	Joback Method
hfus	64.42	kJ/mol	Joback Method
hvap	93.19	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.935		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	750.61	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2955.00		NIST Webbook
tb	973.02	K	Joback Method
tc	1197.14	K	Joback Method
tf	503.29	K	Joback Method
vc	1.563	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.46	J/mol×K	973.02	Joback Method
cpg	1403.49	J/mol×K	1010.37	Joback Method
cpg	1422.90	J/mol×K	1047.73	Joback Method
cpg	1440.75	J/mol×K	1085.08	Joback Method
cpg	1457.13	J/mol×K	1122.43	Joback Method
cpg	1472.09	J/mol×K	1159.79	Joback Method
cpg	1485.71	J/mol×K	1197.14	Joback Method
dvisc	0.0004419	Pa×s	503.29	Joback Method

dvisc	0.0001669	Pa×s	581.58	Joback Method
dvisc	0.0000794	Pa×s	659.87	Joback Method
dvisc	0.0000442	Pa×s	738.15	Joback Method
dvisc	0.0000276	Pa×s	816.44	Joback Method
dvisc	0.0000187	Pa×s	894.73	Joback Method
dvisc	0.0000134	Pa×s	973.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348089&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