Fumaric acid, 2-methylpent-3-yl tridecyl ester

Inchi: InChI=1S/C23H42O4/c1-5-7-8-9-10-11-12-13-14-15-16-19-26-22(24)17-18-23(25)27-21(
InchiKey: YOIKCDKVGCMJKN-ISLYRVAYSA-N
Formula: C23H42O4
SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-249.72	kJ/mol	Joback Method
hf	-900.99	kJ/mol	Joback Method
hfus	54.06	kJ/mol	Joback Method
hvap	84.29	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.375		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	937.49	kPa	Joback Method
rinpol	2572.00		NIST Webbook
rinpol	2572.00		NIST Webbook
tb	881.50	K	Joback Method
tc	1079.40	K	Joback Method
tf	458.21	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.76	J/mol×K	881.50	Joback Method
cpg	1147.77	J/mol×K	914.48	Joback Method
cpg	1165.55	J/mol×K	947.47	Joback Method
cpg	1182.15	J/mol×K	980.45	Joback Method
cpg	1197.61	J/mol×K	1013.43	Joback Method
cpg	1211.97	J/mol×K	1046.42	Joback Method
cpg	1225.26	J/mol×K	1079.40	Joback Method
dvisc	0.0007651	Pa×s	458.21	Joback Method

dvisc	0.0002957	Pa×s	528.76	Joback Method
dvisc	0.0001430	Pa×s	599.31	Joback Method
dvisc	0.0000806	Pa×s	669.86	Joback Method
dvisc	0.0000506	Pa×s	740.40	Joback Method
dvisc	0.0000345	Pa×s	810.95	Joback Method
dvisc	0.0000250	Pa×s	881.50	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=U348770&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