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

Inchi: InChI=1S/C30H56O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-33-29(
InchiKey: OPHRMWIXMXIXEZ-OCOZRVBESA-N
Formula: C30H56O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-190.78	kJ/mol	Joback Method
hf	-1045.47	kJ/mol	Joback Method
hfus	72.19	kJ/mol	Joback Method
hvap	99.87	kJ/mol	Joback Method
log10ws	-9.83		Crippen Method
logp	9.105		Crippen Method
mcvol	444.140	ml/mol	McGowan Method
pc	644.83	kPa	Joback Method
rinpol	3279.00		NIST Webbook
rinpol	3279.00		NIST Webbook
tb	1041.66	K	Joback Method
tc	1298.21	K	Joback Method
tf	537.10	K	Joback Method
vc	1.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.27	J/mol×K	1041.66	Joback Method
cpg	1600.39	J/mol×K	1084.42	Joback Method
cpg	1621.40	J/mol×K	1127.18	Joback Method
cpg	1640.41	J/mol×K	1169.93	Joback Method
cpg	1657.56	J/mol×K	1212.69	Joback Method
cpg	1672.96	J/mol×K	1255.45	Joback Method
cpg	1686.75	J/mol×K	1298.21	Joback Method
dvisc	0.0002861	Pa×s	537.10	Joback Method

dvisc	0.0001064	Pa×s	621.19	Joback Method
dvisc	0.0000501	Pa×s	705.29	Joback Method
dvisc	0.0000277	Pa×s	789.38	Joback Method
dvisc	0.0000172	Pa×s	873.47	Joback Method
dvisc	0.0000116	Pa×s	957.57	Joback Method
dvisc	0.0000083	Pa×s	1041.66	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=U348776&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