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

Inchi: InChI=1S/C30H56O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-33-28(

InchiKey: UWPSFUHXYRHLOJ-OCOZRVBESA-N

Formula: C30H56O4

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

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-185.50	kJ/mol	Joback Method
hf	-1048.94	kJ/mol	Joback Method
hfus	68.30	kJ/mol	Joback Method
hvap	98.96	kJ/mol	Joback Method
log10ws	-9.83		Crippen Method
logp	9.105		Crippen Method
mcvol	444.140	ml/mol	McGowan Method
pc	648.45	kPa	Joback Method
rinpol	3247.00		NIST Webbook
rinpol	3247.00		NIST Webbook
tb	1038.87	K	Joback Method
tc	1289.47	K	Joback Method
tf	554.52	K	Joback Method
vc	1.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.69	J/mol×K	1038.87	Joback Method
cpg	1675.29	J/mol×K	1247.71	Joback Method
cpg	1658.58	J/mol×K	1205.94	Joback Method
cpg	1640.51	J/mol×K	1164.17	Joback Method
cpg	1620.93	J/mol×K	1122.40	Joback Method
cpg	1599.71	J/mol×K	1080.64	Joback Method
cpg	1690.79	J/mol×K	1289.47	Joback Method
dvisc	0.0000068	Pa×s	1038.87	Joback Method

dvisc	0.0000096	Pa×s	958.14	Joback Method
dvisc	0.0000142	Pa×s	877.42	Joback Method
dvisc	0.0000229	Pa×s	796.69	Joback Method
dvisc	0.0000410	Pa×s	715.97	Joback Method
dvisc	0.0000853	Pa×s	635.25	Joback Method
dvisc	0.0002197	Pa×s	554.52	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=U348719&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