Fumaric acid, eicosyl 3-heptyl ester

Inchi: InChI=1S/C31H58O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-28-34-30
InchiKey: WSEQFJATTAZGKE-CYYJNZCTSA-N
Formula: C31H58O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCCC
Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-179.92	kJ/mol	Joback Method
hf	-1060.83	kJ/mol	Joback Method
hfus	78.30	kJ/mol	Joback Method
hvap	102.48	kJ/mol	Joback Method
log10ws	-10.49		Crippen Method
logp	9.639		Crippen Method
mcvol	458.230	ml/mol	McGowan Method
pc	612.08	kPa	Joback Method
rinpol	3380.00		NIST Webbook
tb	1064.98	K	Joback Method
tc	1338.92	K	Joback Method
tf	563.37	K	Joback Method
vc	1.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1642.70	J/mol×K	1064.98	Joback Method
cpg	1742.40	J/mol×K	1293.26	Joback Method
cpg	1726.56	J/mol×K	1247.61	Joback Method
cpg	1708.83	J/mol×K	1201.95	Joback Method
cpg	1689.04	J/mol×K	1156.29	Joback Method
cpg	1667.05	J/mol×K	1110.64	Joback Method
cpg	1756.51	J/mol×K	1338.92	Joback Method
dvisc	0.0000078	Pa×s	1064.98	Joback Method
dvisc	0.0000107	Pa×s	981.38	Joback Method

dvisc	0.0000156	Pa×s	897.78	Joback Method
dvisc	0.0000246	Pa×s	814.17	Joback Method
dvisc	0.0000431	Pa×s	730.57	Joback Method
dvisc	0.0000870	Pa×s	646.97	Joback Method
dvisc	0.0002169	Pa×s	563.37	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=U348697&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