Fumaric acid, tetradec-3-enyl tridecyl ester

Inchi: InChI=1S/C31H56O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-29-35-31(33)27-26-30(32)34-
InchiKey: HBJVRZVOMKFHMS-LSSFEAIKSA-N
Formula: C31H56O4
SMILES: CCCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-97.26	kJ/mol	Joback Method
hf	-938.33	kJ/mol	Joback Method
hfus	82.02	kJ/mol	Joback Method
hvap	102.83	kJ/mol	Joback Method
log10ws	-10.23		Crippen Method
logp	9.417		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
pc	625.63	kPa	Joback Method
rinpol	3508.00		NIST Webbook
tb	1069.58	K	Joback Method
tc	1342.42	K	Joback Method
tf	573.29	K	Joback Method
vc	1.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1614.23	J/mol×K	1069.58	Joback Method
cpg	1718.28	J/mol×K	1296.95	Joback Method
cpg	1700.74	J/mol×K	1251.47	Joback Method
cpg	1681.75	J/mol×K	1206.00	Joback Method
cpg	1661.12	J/mol×K	1160.53	Joback Method
cpg	1638.68	J/mol×K	1115.05	Joback Method
cpg	1734.55	J/mol×K	1342.42	Joback Method
dvisc	0.0000076	Pa×s	1069.58	Joback Method
dvisc	0.0000103	Pa×s	986.86	Joback Method

dvisc	0.0000148	Pa×s	904.15	Joback Method
dvisc	0.0000228	Pa×s	821.43	Joback Method
dvisc	0.0000390	Pa×s	738.72	Joback Method
dvisc	0.0000761	Pa×s	656.00	Joback Method
dvisc	0.0001801	Pa×s	573.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348844&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

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