

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-LSSF EAIKSA-N
Formula: C31H56O4
SMILES: CCCCCCCCCC=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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000148	Paxs	904.15	Joback Method
dvisc	0.0000228	Paxs	821.43	Joback Method
dvisc	0.0000390	Paxs	738.72	Joback Method
dvisc	0.0000761	Paxs	656.00	Joback Method
dvisc	0.0001801	Paxs	573.29	Joback Method

Sources

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=U348844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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