

Fumaric acid, dodecyl tetradec-3-enyl ester

Inchi:	InChI=1S/C30H54O4/c1-3-5-7-9-11-13-15-16-18-20-22-24-28-34-30(32)26-25-29(31)33-
InchiKey:	YQDQWBFXNCSFPC-BMRAXTPNSA-N
Formula:	C30H54O4
SMILES:	CCCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	478.75

Physical Properties

Property code	Value	Unit	Source
gf	-105.68	kJ/mol	Joback Method
hf	-917.69	kJ/mol	Joback Method
hfus	79.43	kJ/mol	Joback Method
hvap	100.60	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	9.027		Crippen Method
mvol	439.840	ml/mol	McGowan Method
pc	656.79	kPa	Joback Method
rinpol	3405.00		NIST Webbook
rinpol	3405.00		NIST Webbook
tb	1046.70	K	Joback Method
tc	1305.52	K	Joback Method
tf	562.02	K	Joback Method
vc	1.724	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.54	J/molxK	1046.70	Joback Method
cpg	1571.96	J/molxK	1089.84	Joback Method
cpg	1593.55	J/molxK	1132.97	Joback Method
cpg	1613.46	J/molxK	1176.11	Joback Method
cpg	1631.83	J/molxK	1219.25	Joback Method
cpg	1648.81	J/molxK	1262.38	Joback Method
cpg	1664.56	J/molxK	1305.52	Joback Method
dvisc	0.0002071	Paxs	562.02	Joback Method

dvisc	0.0000881	Paxs	642.80	Joback Method
dvisc	0.0000453	Paxs	723.58	Joback Method
dvisc	0.0000267	Paxs	804.36	Joback Method
dvisc	0.0000173	Paxs	885.14	Joback Method
dvisc	0.0000120	Paxs	965.92	Joback Method
dvisc	0.0000089	Paxs	1046.70	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=U348843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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