

Fumaric acid, nonyl tetradec-3-enyl ester

Inchi:	InChI=1S/C27H48O4/c1-3-5-7-9-11-12-13-14-15-17-19-21-25-31-27(29)23-22-26(28)30-
InchiKey:	UDHQAQGBJFMCBK-OLENSVKVSA-N
Formula:	C27H48O4
SMILES:	CCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	436.67

Physical Properties

Property code	Value	Unit	Source
gf	-130.94	kJ/mol	Joback Method
hf	-855.77	kJ/mol	Joback Method
hfus	71.66	kJ/mol	Joback Method
hvap	93.92	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.857		Crippen Method
mvol	397.570	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	3102.00		NIST Webbook
rinpol	3102.00		NIST Webbook
tb	978.06	K	Joback Method
tc	1203.84	K	Joback Method
tf	528.21	K	Joback Method
vc	1.556	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.80	J/molxK	978.06	Joback Method
cpg	1374.69	J/molxK	1015.69	Joback Method
cpg	1394.13	J/molxK	1053.32	Joback Method
cpg	1412.23	J/molxK	1090.95	Joback Method
cpg	1429.06	J/molxK	1128.58	Joback Method
cpg	1444.72	J/molxK	1166.21	Joback Method
cpg	1459.30	J/molxK	1203.84	Joback Method
dvisc	0.0003108	Paxs	528.21	Joback Method

dvisc	0.0001350	Paxs	603.19	Joback Method
dvisc	0.0000706	Paxs	678.16	Joback Method
dvisc	0.0000419	Paxs	753.13	Joback Method
dvisc	0.0000274	Paxs	828.11	Joback Method
dvisc	0.0000192	Paxs	903.09	Joback Method
dvisc	0.0000142	Paxs	978.06	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=U348840&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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