

Dodecanoic acid octadeca-9,12-dienyl ester, Z

Inchi:	InChI=1S/C30H56O2/c1-3-5-7-9-11-13-14-15-16-17-18-19-21-23-25-27-29-32-30(31)28-
InchiKey:	HHGLCKLXHVTCRU-FYNKLMPSA-N
Formula:	C30H56O2
SMILES:	CCCCC=CCC=CCCCCCCCCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	448.76

Physical Properties

Property code	Value	Unit	Source
gf	128.24	kJ/mol	Joback Method
hf	-672.89	kJ/mol	Joback Method
hfus	76.65	kJ/mol	Joback Method
hvap	91.45	kJ/mol	Joback Method
log10ws	-10.95		Crippen Method
logp	10.264		Crippen Method
mvol	432.400	ml/mol	McGowan Method
pc	641.57	kPa	Joback Method
rinpol	3118.21		NIST Webbook
tb	970.41	K	Joback Method
tc	1199.11	K	Joback Method
tf	489.86	K	Joback Method
vc	1.700	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1493.99	J/molxK	970.41	Joback Method
cpg	1604.77	J/molxK	1161.00	Joback Method
cpg	1585.06	J/molxK	1122.88	Joback Method
cpg	1564.25	J/molxK	1084.76	Joback Method
cpg	1542.22	J/molxK	1046.64	Joback Method
cpg	1518.84	J/molxK	1008.53	Joback Method
cpg	1623.51	J/molxK	1199.11	Joback Method
dvisc	0.0000130	Paxs	970.41	Joback Method
dvisc	0.0000179	Paxs	890.32	Joback Method

dvisc	0.0000262	Paxs	810.23	Joback Method
dvisc	0.0000419	Paxs	730.13	Joback Method
dvisc	0.0000750	Paxs	650.04	Joback Method
dvisc	0.0001583	Paxs	569.95	Joback Method
dvisc	0.0004267	Paxs	489.86	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=R437042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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