

Dodecanoic acid tetradec-9-enyl ester, Z

Inchi:	InChI=1S/C26H50O2/c1-3-5-7-9-11-13-14-15-17-19-21-23-25-28-26(27)24-22-20-18-16-
InchiKey:	FCFZEKPMNDZSLV-PKQNBQFBNSA-N
Formula:	C26H50O2
SMILES:	CCCCC=CCCCCCCCCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	394.67

Physical Properties

Property code	Value	Unit	Source
gf	14.34	kJ/mol	Joback Method
hf	-707.55	kJ/mol	Joback Method
hfus	66.09	kJ/mol	Joback Method
hvap	82.58	kJ/mol	Joback Method
log10ws	-9.42		Crippen Method
logp	8.928		Crippen Method
mvol	380.340	ml/mol	McGowan Method
pc	764.79	kPa	Joback Method
rinpol	2743.36		NIST Webbook
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tb	874.73	K	Joback Method
tc	1071.62	K	Joback Method
tf	449.86	K	Joback Method
vc	1.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1259.27	J/molxK	874.73	Joback Method
cpg	1281.50	J/molxK	907.55	Joback Method
cpg	1302.48	J/molxK	940.36	Joback Method
cpg	1322.28	J/molxK	973.18	Joback Method
cpg	1340.96	J/molxK	1005.99	Joback Method
cpg	1358.57	J/molxK	1038.81	Joback Method
cpg	1375.17	J/molxK	1071.62	Joback Method
dvisc	0.0007748	Paxs	449.86	Joback Method

dvisc	0.0003032	Paxs	520.67	Joback Method
dvisc	0.0001486	Paxs	591.48	Joback Method
dvisc	0.0000848	Paxs	662.29	Joback Method
dvisc	0.0000539	Paxs	733.11	Joback Method
dvisc	0.0000371	Paxs	803.92	Joback Method
dvisc	0.0000272	Paxs	874.73	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=R436569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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