

Dodecanoic acid hexadec-9-enyl ester, Z

Inchi:	InChI=1S/C28H54O2/c1-3-5-7-9-11-13-14-15-16-17-19-21-23-25-27-30-28(29)26-24-22-
InchiKey:	IJBWCQYSLOUKSH-BUHFOSPRSA-N
Formula:	C28H54O2
SMILES:	CCCCCCC=CCCCCCCCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	422.73

Physical Properties

Property code	Value	Unit	Source
gf	31.18	kJ/mol	Joback Method
hf	-748.83	kJ/mol	Joback Method
hfus	71.27	kJ/mol	Joback Method
hvap	87.04	kJ/mol	Joback Method
log10ws	-10.26		Crippen Method
logp	9.708		Crippen Method
mvol	408.520	ml/mol	McGowan Method
pc	689.61	kPa	Joback Method
rinpol	2932.01		NIST Webbook
rinpol	2932.01		NIST Webbook
tb	920.49	K	Joback Method
tc	1132.10	K	Joback Method
tf	472.40	K	Joback Method
vc	1.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1389.38	J/molxK	920.49	Joback Method
cpg	1413.09	J/molxK	955.76	Joback Method
cpg	1435.36	J/molxK	991.03	Joback Method
cpg	1456.28	J/molxK	1026.29	Joback Method
cpg	1475.93	J/molxK	1061.56	Joback Method
cpg	1494.38	J/molxK	1096.83	Joback Method
cpg	1511.71	J/molxK	1132.10	Joback Method
dvisc	0.0005975	Paxs	472.40	Joback Method

dvisc	0.0002308	Paxs	547.08	Joback Method
dvisc	0.0001121	Paxs	621.76	Joback Method
dvisc	0.0000635	Paxs	696.44	Joback Method
dvisc	0.0000402	Paxs	771.13	Joback Method
dvisc	0.0000276	Paxs	845.81	Joback Method
dvisc	0.0000201	Paxs	920.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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