

Docosanoic acid octadec-9-enyl ester, Z

Inchi:	InChI=1S/C40H78O2/c1-3-5-7-9-11-13-15-17-19-21-22-23-24-26-28-30-32-34-36-38-40(
InchiKey:	AOXNDJKHXBKZBT-CZIZESTLSA-N
Formula:	C40H78O2
SMILES:	CCCCCCCCC=CCCCCCCCCOC(=O)CCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	591.05

Physical Properties

Property code	Value	Unit	Source
gf	132.22	kJ/mol	Joback Method
hf	-996.51	kJ/mol	Joback Method
hfus	102.34	kJ/mol	Joback Method
hvap	113.75	kJ/mol	Joback Method
log10ws	-15.28		Crippen Method
logp	14.389		Crippen Method
mvol	577.600	ml/mol	McGowan Method
pc	406.48	kPa	Joback Method
rinpol	4124.32		NIST Webbook
rinpol	4124.32		NIST Webbook
tb	1195.05	K	Joback Method
tc	1628.18	K	Joback Method
tf	607.64	K	Joback Method
vc	2.280	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2203.01	J/molxK	1195.05	Joback Method
cpg	2245.29	J/molxK	1267.24	Joback Method
cpg	2283.38	J/molxK	1339.43	Joback Method
cpg	2318.30	J/molxK	1411.62	Joback Method
cpg	2351.05	J/molxK	1483.81	Joback Method
cpg	2382.65	J/molxK	1555.99	Joback Method
cpg	2414.11	J/molxK	1628.18	Joback Method
dvisc	0.0001045	Paxs	607.64	Joback Method

dvisc	0.0000381	Paxs	705.54	Joback Method
dvisc	0.0000177	Paxs	803.44	Joback Method
dvisc	0.0000098	Paxs	901.35	Joback Method
dvisc	0.0000060	Paxs	999.25	Joback Method
dvisc	0.0000041	Paxs	1097.15	Joback Method
dvisc	0.0000029	Paxs	1195.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R437037&Units=SI

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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