Hexadec-9-enoic acid dodecyl ester, Z

Inchi: InChI=1S/C28H54O2/c1-3-5-7-9-11-13-15-16-17-18-20-22-24-26-28(29)30-27-25-23-21-
InchiKey: CDXFYPWJGOODOG-SQFISAMPSA-N
Formula: C28H54O2
SMILES: CCCCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCC
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
mcvol	408.520	ml/mol	McGowan Method
pc	689.61	kPa	Joback Method
rinpol	2931.17		NIST Webbook
rinpol	2931.17		NIST Webbook
tb	920.49	K	Joback Method
tc	1132.10	K	Joback Method
tf	472.40	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1389.38	J/mol×K	920.49	Joback Method
cpg	1494.38	J/mol×K	1096.83	Joback Method
cpg	1475.93	J/mol×K	1061.56	Joback Method
cpg	1456.28	J/mol×K	1026.29	Joback Method
cpg	1435.36	J/mol×K	991.03	Joback Method
cpg	1413.09	J/mol×K	955.76	Joback Method
cpg	1511.71	J/mol×K	1132.10	Joback Method
dvisc	0.0000201	Pa×s	920.49	Joback Method

dvisc	0.0000276	Pa×s	845.81	Joback Method
dvisc	0.0000402	Pa×s	771.13	Joback Method
dvisc	0.0000635	Pa×s	696.44	Joback Method
dvisc	0.0001121	Pa×s	621.76	Joback Method
dvisc	0.0002308	Pa×s	547.08	Joback Method
dvisc	0.0005975	Pa×s	472.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R436465&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