

Tetradec-9-enoic acid dodecyl ester, Z

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C26H50O2/c1-3-5-7-9-11-13-15-16-18-20-22-24-26(27)28-25-23-21-19-17-14-

BNVVXPRRISYSOG-LUAWRHEFSA-N

C26H50O2

CCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCCC

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
mcvol	380.340	ml/mol	McGowan Method
pc	764.79	kPa	Joback Method
rinpol	2742.52		NIST Webbook
rinpol	2742.52		NIST Webbook
tb	874.73	K	Joback Method
tc	1071.62	K	Joback Method
tf	449.86	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003032	Pa×s	520.67	Joback Method
dvisc	0.0001486	Pa×s	591.48	Joback Method
dvisc	0.0000848	Pa×s	662.29	Joback Method
dvisc	0.0000539	Pa×s	733.11	Joback Method
dvisc	0.0000371	Pa×s	803.92	Joback Method
dvisc	0.0000272	Pa×s	874.73	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=R436450&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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