

Tetracosanoic acid, propyl ester

Other names:	propyl tetracosanoate
Inchi:	InChI=1S/C27H54O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	KNLZZQYOTJRNTD-UHFFFAOYSA-N
Formula:	C27H54O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]:	410.72

Physical Properties

Property code	Value	Unit	Source
gf	-57.46	kJ/mol	Joback Method
hf	-845.41	kJ/mol	Joback Method
hfus	68.47	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-9.99		Crippen Method
logp	9.542		Crippen Method
mcvol	398.730	ml/mol	McGowan Method
pc	705.83	kPa	Joback Method
rinpol	2877.44		NIST Webbook
rinpol	2877.44		NIST Webbook
tb	893.45	K	Joback Method
tc	1097.77	K	Joback Method
tf	466.21	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.54	J/molxK	893.45	Joback Method
cpg	1454.85	J/molxK	1063.71	Joback Method
cpg	1436.68	J/molxK	1029.66	Joback Method
cpg	1417.22	J/molxK	995.61	Joback Method
cpg	1396.42	J/molxK	961.56	Joback Method
cpg	1374.21	J/molxK	927.50	Joback Method
cpg	1471.80	J/molxK	1097.77	Joback Method

dvisc	0.0000268	Paxs	893.45	Joback Method
dvisc	0.0000366	Paxs	822.24	Joback Method
dvisc	0.0000530	Paxs	751.04	Joback Method
dvisc	0.0000831	Paxs	679.83	Joback Method
dvisc	0.0001446	Paxs	608.62	Joback Method
dvisc	0.0002915	Paxs	537.42	Joback Method
dvisc	0.0007281	Paxs	466.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405157&Units=SI
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

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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