Hexacosanoic acid, propyl ester

Other names: Propyl hexacosanoate
Inchi: InChI=1S/C29H58O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: NTWJOTULVRNHFR-UHFFFAOYSA-N
Formula: C29H58O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 438.77
CAS: 40710-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-40.62	kJ/mol	Joback Method
hf	-886.69	kJ/mol	Joback Method
hfus	73.65	kJ/mol	Joback Method
hvap	89.30	kJ/mol	Joback Method
log10ws	-10.82		Crippen Method
logp	10.322		Crippen Method
mcvol	426.910	ml/mol	McGowan Method
pc	638.98	kPa	Joback Method
rinpol	3078.35		NIST Webbook
rinpol	3078.35		NIST Webbook
tb	939.21	K	Joback Method
tc	1161.87	K	Joback Method
tf	488.75	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.38	J/mol×K	939.21	Joback Method
cpg	1507.73	J/mol×K	976.32	Joback Method
cpg	1531.33	J/mol×K	1013.43	Joback Method
cpg	1553.27	J/mol×K	1050.54	Joback Method
cpg	1573.64	J/mol×K	1087.65	Joback Method
cpg	1592.51	J/mol×K	1124.76	Joback Method

cpg	1609.96	J/mol×K	1161.87	Joback Method
dvisc	0.0005585	Pa×s	488.75	Joback Method
dvisc	0.0002206	Pa×s	563.83	Joback Method
dvisc	0.0001084	Pa×s	638.90	Joback Method
dvisc	0.0000618	Pa×s	713.98	Joback Method
dvisc	0.0000393	Pa×s	789.06	Joback Method
dvisc	0.0000270	Pa×s	864.13	Joback Method
dvisc	0.0000197	Pa×s	939.21	Joback Method

Sources

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=C40710381&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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