

propyl dotriacontanoate

Inchi: InChI=1S/C35H70O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: XFCFEODJNQMKLS-UHFFFAOYSA-N
Formula: C35H70O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 522.93

Physical Properties

Property code	Value	Unit	Source
gf	9.90	kJ/mol	Joback Method
hf	-1010.53	kJ/mol	Joback Method
hfus	89.19	kJ/mol	Joback Method
hvap	102.66	kJ/mol	Joback Method
log10ws	-13.34		Crippen Method
logp	12.662		Crippen Method
mvol	511.450	ml/mol	McGowan Method
pc	486.88	kPa	Joback Method
rinpol	3681.16		NIST Webbook
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tb	1076.49	K	Joback Method
tc	1389.63	K	Joback Method
tf	556.37	K	Joback Method
vc	2.019	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1886.65	J/molxK	1076.49	Joback Method
cpg	2019.77	J/molxK	1337.44	Joback Method
cpg	1998.46	J/molxK	1285.25	Joback Method
cpg	1974.78	J/molxK	1233.06	Joback Method
cpg	1948.44	J/molxK	1180.87	Joback Method
cpg	1919.16	J/molxK	1128.68	Joback Method
cpg	2039.01	J/molxK	1389.63	Joback Method
dvisc	0.0000076	Paxs	1076.49	Joback Method

dvisc	0.0000104	Paxs	989.80	Joback Method
dvisc	0.0000154	Paxs	903.12	Joback Method
dvisc	0.0000245	Paxs	816.43	Joback Method
dvisc	0.0000437	Paxs	729.74	Joback Method
dvisc	0.0000910	Paxs	643.06	Joback Method
dvisc	0.0002385	Paxs	556.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R438005&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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