triacontyl hexanoate

Inchi: InChI=1S/C36H72O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: YQUUPVOQWDIUFK-UHFFFAOYSA-N
Formula: C36H72O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]: 536.96

Physical Properties

Property code	Value	Unit	Source
gf	18.32	kJ/mol	Joback Method
hf	-1031.17	kJ/mol	Joback Method
hfus	91.78	kJ/mol	Joback Method
hvap	104.89	kJ/mol	Joback Method
log10ws	-13.75		Crippen Method
logp	13.053		Crippen Method
mcvol	525.540	ml/mol	McGowan Method
pc	466.89	kPa	Joback Method
rinpol	3772.13		NIST Webbook
tb	1099.37	K	Joback Method
tc	1434.20	K	Joback Method
tf	567.64	K	Joback Method
vc	2.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1954.91	J/mol×K	1099.37	Joback Method
cpg	1989.00	J/mol×K	1155.17	Joback Method
cpg	2019.47	J/mol×K	1210.98	Joback Method
cpg	2046.69	J/mol×K	1266.78	Joback Method
cpg	2071.04	J/mol×K	1322.59	Joback Method
cpg	2092.87	J/mol×K	1378.39	Joback Method
cpg	2112.57	J/mol×K	1434.20	Joback Method
dvisc	0.0002056	Pa×s	567.64	Joback Method
dvisc	0.0000781	Pa×s	656.26	Joback Method

dvisc	0.0000374	Pa×s	744.88	Joback Method
dvisc	0.0000209	Pa×s	833.50	Joback Method
dvisc	0.0000131	Pa×s	922.13	Joback Method
dvisc	0.0000089	Pa×s	1010.75	Joback Method
dvisc	0.0000064	Pa×s	1099.37	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=R438085&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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