

triacontyl hexanoate

Inchi: InChI=1S/C36H72O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: YQUUPVOQWDIUFK-UHFFFAOYSA-N
Formula: C36H72O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=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/molxK	1099.37	Joback Method
cpg	1989.00	J/molxK	1155.17	Joback Method
cpg	2019.47	J/molxK	1210.98	Joback Method
cpg	2046.69	J/molxK	1266.78	Joback Method
cpg	2071.04	J/molxK	1322.59	Joback Method
cpg	2092.87	J/molxK	1378.39	Joback Method
cpg	2112.57	J/molxK	1434.20	Joback Method
dvisc	0.0002056	Paxs	567.64	Joback Method
dvisc	0.0000781	Paxs	656.26	Joback Method

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