Triacontyl acetate

Other names: n-Triacontyl acetate
1-Triacontanol, acetate
Melissyl acetate
Inchi: InChI=1S/C32H64O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: OVQVOKLGCDAZBX-UHFFFAOYSA-N
Formula: C32H64O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 480.85
CAS: 41755-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-15.36	kJ/mol	Joback Method
hf	-948.61	kJ/mol	Joback Method
hfus	81.42	kJ/mol	Joback Method
hvap	95.98	kJ/mol	Joback Method
log10ws	-12.08		Crippen Method
logp	11.492		Crippen Method
mcvol	469.180	ml/mol	McGowan Method
pc	555.20	kPa	Joback Method
rinpol	3412.20		NIST Webbook
rinpol	3398.06		NIST Webbook
tb	1007.85	K	Joback Method
tc	1268.18	K	Joback Method
tf	522.56	K	Joback Method
vc	1.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1683.18	J/mol×K	1007.85	Joback Method
cpg	1803.68	J/mol×K	1224.79	Joback Method
cpg	1783.67	J/mol×K	1181.40	Joback Method
cpg	1761.76	J/mol×K	1138.01	Joback Method

cpg	1737.81	J/mol×K	1094.63	Joback Method
cpg	1711.67	J/mol×K	1051.24	Joback Method
cpg	1821.94	J/mol×K	1268.18	Joback Method
dvisc	0.0000123	Pa×s	1007.85	Joback Method
dvisc	0.0000169	Pa×s	926.97	Joback Method
dvisc	0.0000247	Pa×s	846.09	Joback Method
dvisc	0.0000392	Pa×s	765.20	Joback Method
dvisc	0.0000693	Pa×s	684.32	Joback Method
dvisc	0.0001429	Pa×s	603.44	Joback Method
dvisc	0.0003683	Pa×s	522.56	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41755582&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from: