

1-Oleoyl-3-acetyl-glycerol

Inchi:	InChI=1S/C23H42O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23(26)28-20-22(25)
InchiKey:	UDOOJTYHKCEVFS-KHPPLWFESA-N
Formula:	C23H42O5
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCC(O)COC(C)=O
Mol. weight [g/mol]:	398.58

Physical Properties

Property code	Value	Unit	Source
gf	-384.10	kJ/mol	Joback Method
hf	-1047.94	kJ/mol	Joback Method
hfus	61.67	kJ/mol	Joback Method
hvap	101.35	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.491		Crippen Method
mvol	351.380	ml/mol	McGowan Method
pc	987.64	kPa	Joback Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		NIST Webbook
tb	974.12	K	Joback Method
tc	1200.65	K	Joback Method
tf	534.03	K	Joback Method
vc	1.365	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.07	J/molxK	974.12	Joback Method
cpg	1273.43	J/molxK	1162.89	Joback Method
cpg	1260.79	J/molxK	1125.14	Joback Method
cpg	1246.89	J/molxK	1087.38	Joback Method
cpg	1231.68	J/molxK	1049.63	Joback Method
cpg	1215.10	J/molxK	1011.87	Joback Method
cpg	1284.89	J/molxK	1200.65	Joback Method
dvisc	0.0000034	Paxs	974.12	Joback Method

dvisc	0.0000052	Paxs	900.77	Joback Method
dvisc	0.0000084	Paxs	827.42	Joback Method
dvisc	0.0000151	Paxs	754.07	Joback Method
dvisc	0.0000306	Paxs	680.73	Joback Method
dvisc	0.0000735	Paxs	607.38	Joback Method
dvisc	0.0002249	Paxs	534.03	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=R501138&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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