

1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate

Inchi:	InChI=1S/C21H40O5/c1-3-5-7-9-10-12-14-16-21(24)26-19(17-22)18-25-20(23)15-13-11-
InchiKey:	YOYOQXRPUDEPAK-UHFFFAOYSA-N
Formula:	C21H40O5
SMILES:	CCCCCCCCC(=O)OC(CO)COC(=O)CCCCCCC
Mol. weight [g/mol]:	372.54
CAS:	177717-46-3

Physical Properties

Property code	Value	Unit	Source
gf	-481.16	kJ/mol	Joback Method
hf	-1123.88	kJ/mol	Joback Method
hfus	56.28	kJ/mol	Joback Method
hvap	96.94	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.935		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2560.60		NIST Webbook
rinpol	2560.60		NIST Webbook
tb	924.20	K	Joback Method
tc	1134.71	K	Joback Method
tf	516.57	K	Joback Method
vc	1.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.15	J/molxK	924.20	Joback Method
cpg	1118.52	J/molxK	959.28	Joback Method
cpg	1134.54	J/molxK	994.37	Joback Method
cpg	1149.24	J/molxK	1029.45	Joback Method
cpg	1162.66	J/molxK	1064.54	Joback Method
cpg	1174.83	J/molxK	1099.62	Joback Method
cpg	1185.78	J/molxK	1134.71	Joback Method

dvisc	0.0003392	Paxs	516.57	Joback Method
dvisc	0.0001157	Paxs	584.51	Joback Method
dvisc	0.0000493	Paxs	652.45	Joback Method
dvisc	0.0000247	Paxs	720.38	Joback Method
dvisc	0.0000140	Paxs	788.32	Joback Method
dvisc	0.0000086	Paxs	856.26	Joback Method
dvisc	0.0000057	Paxs	924.20	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=C177717463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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