2-Hydroxy-3-(octanoyloxy)propyl decanoate

Other names: 2-Hydroxy-3-(octanoyloxy)propyl decanoate
Inchi: InChI=1S/C21H40O5/c1-3-5-7-9-10-12-14-16-21(24)26-18-19(22)17-25-20(23)15-13-11-
InchiKey: AMRVOUCEFGMNBS-UHFFFAOYSA-N
Formula: C21H40O5
SMILES: CCCCCCCCCC(=O)OCC(O)COC(=O)CCCCCCC
Mol. weight [g/mol]: 372.55

Physical Properties

Property code	Value	Unit	Source
af	1.2240		Cheméo Relay (1.0)
hf	-1277.54	kJ/mol	Cheméo Relay (1.0)
hfus	56.28	kJ/mol	Joback Method
hvap	120.36	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	Cheméo Relay (1.0)
log10ws	-4.93		Cheméo Relay (1.0)
logp	4.935		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2572.40		NIST Webbook
rinpol	2572.40		NIST Webbook
tb	645.17	K	Cheméo Relay (1.0)
tc	820.74	K	Cheméo Relay (1.0)
tf	316.70	K	Cheméo Relay (1.0)
vc	1.269	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	1118.52	J/mol×K	959.28	Joback Method
dvisc	0.0000247	Pa×s	720.38	Joback Method
dvisc	0.0000057	Pa×s	924.20	Joback Method
dvisc	0.0000086	Pa×s	856.26	Joback Method
dvisc	0.0000140	Pa×s	788.32	Joback Method
dvisc	0.0003392	Pa×s	516.57	Joback Method
dvisc	0.0000493	Pa×s	652.45	Joback Method
dvisc	0.0001157	Pa×s	584.51	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93980848&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

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