

2-(Octanoyloxy)propane-1,3-diyl bis(decanoate)

Inchi:	InChI=1S/C31H58O6/c1-4-7-10-13-15-18-20-23-29(32)35-26-28(37-31(34)25-22-17-12-9
InchiKey:	CYHAOTQWWRWBAF-UHFFFAOYSA-N
Formula:	C31H58O6
SMILES:	CCCCCCCCC(=O)OCC(COC(=O)CCCCCCCC)OC(=O)CCCCCCC
Mol. weight [g/mol]:	526.79
CAS:	33368-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-494.06	kJ/mol	Joback Method
hf	-1422.85	kJ/mol	Joback Method
hfus	80.88	kJ/mol	Joback Method
hvap	111.68	kJ/mol	Joback Method
log10ws	-9.50		Crippen Method
logp	8.627		Crippen Method
mcvol	469.970	ml/mol	McGowan Method
pc	610.27	kPa	Joback Method
rinpol	3309.70		NIST Webbook
rinpol	3309.70		NIST Webbook
tb	1137.11	K	Joback Method
tc	1459.53	K	Joback Method
tf	640.61	K	Joback Method
vc	1.837	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1713.18	J/molxK	1137.11	Joback Method
cpg	1777.97	J/molxK	1405.79	Joback Method
cpg	1772.30	J/molxK	1352.06	Joback Method
cpg	1763.15	J/molxK	1298.32	Joback Method
cpg	1750.34	J/molxK	1244.58	Joback Method
cpg	1733.74	J/molxK	1190.85	Joback Method
cpg	1780.30	J/molxK	1459.53	Joback Method

dvisc	0.0000059	Paxs	1137.11	Joback Method
dvisc	0.0000079	Paxs	1054.36	Joback Method
dvisc	0.0000113	Paxs	971.61	Joback Method
dvisc	0.0000172	Paxs	888.86	Joback Method
dvisc	0.0000285	Paxs	806.11	Joback Method
dvisc	0.0000530	Paxs	723.36	Joback Method
dvisc	0.0001157	Paxs	640.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33368864&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

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