2-(2-[(9Z)-9-octadecenoyloxy]ethoxy)ethyl (9z)-9-octadecenoate

Other names: oxydi-2,1-ethanediyl dioleate
Inchi: InChI=1S/C40H74O5/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-39(41)44-37-35-
InchiKey: HJRDNARELSKHEF-CLFAGFIQSA-N
Formula: C40H74O5
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCCOCCOC(=O)CCCCCCCC=CCCCCCCCC
Mol. weight [g/mol]: 635.01
CAS: 21209-30-3

Physical Properties

Property code	Value	Unit	Source
gf	-126.48	kJ/mol	Joback Method
hf	-1256.31	kJ/mol	Joback Method
hfus	106.52	kJ/mol	Joback Method
hvap	125.27	kJ/mol	Joback Method
log10ws	-13.09		Crippen Method
logp	12.164		Crippen Method
mcvol	586.610	ml/mol	McGowan Method
pc	420.09	kPa	Joback Method
tb	1297.92	K	Joback Method
tc	1830.91	K	Joback Method
tf	696.95	K	Joback Method
vc	2.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2240.22	J/mol×K	1297.92	Joback Method
cpg	2276.11	J/mol×K	1386.75	Joback Method
cpg	2306.00	J/mol×K	1475.58	Joback Method
cpg	2331.47	J/mol×K	1564.41	Joback Method
cpg	2354.10	J/mol×K	1653.25	Joback Method
cpg	2375.49	J/mol×K	1742.08	Joback Method
cpg	2397.22	J/mol×K	1830.91	Joback Method
dvisc	0.0000315	Pa×s	696.95	Joback Method

dvisc	0.0000130	Pa×s	797.11	Joback Method
dvisc	0.0000066	Pa×s	897.27	Joback Method
dvisc	0.0000038	Pa×s	997.43	Joback Method
dvisc	0.0000024	Pa×s	1097.60	Joback Method
dvisc	0.0000017	Pa×s	1197.76	Joback Method
dvisc	0.0000012	Pa×s	1297.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21209303&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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