Eicosanoic acid, eicosyl ester

Other names: Eicosyl eicosanoate
eicosanyl eicosanoate
icosyl icosanoate
Inchi: InChI=1S/C40H80O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-42-40(
InchiKey: VJFBRZCPEBSUHG-UHFFFAOYSA-N
Formula: C40H80O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 593.06
CAS: 22432-80-0

Physical Properties

Property code	Value	Unit	Source
gf	52.00	kJ/mol	Joback Method
hf	-1113.73	kJ/mol	Joback Method
hfus	102.14	kJ/mol	Joback Method
hvap	113.79	kJ/mol	Joback Method
log10ws	-15.43		Crippen Method
logp	14.613		Crippen Method
mcvol	581.900	ml/mol	McGowan Method
pc	398.09	kPa	Joback Method
rinpol	4146.16		NIST Webbook
rinpol	4146.16		NIST Webbook
tb	1190.89	K	Joback Method
tc	1638.25	K	Joback Method
tf	612.72	K	Joback Method
vc	2.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2229.58	J/mol×K	1190.89	Joback Method
cpg	2271.31	J/mol×K	1265.45	Joback Method
cpg	2307.48	J/mol×K	1340.01	Joback Method
cpg	2339.08	J/mol×K	1414.57	Joback Method

cpg	2367.11	J/mol×K	1489.13	Joback Method
cpg	2392.58	J/mol×K	1563.69	Joback Method
cpg	2416.46	J/mol×K	1638.25	Joback Method
dvisc	0.0001118	Pa×s	612.72	Joback Method
dvisc	0.0000417	Pa×s	709.08	Joback Method
dvisc	0.0000197	Pa×s	805.44	Joback Method
dvisc	0.0000109	Pa×s	901.80	Joback Method
dvisc	0.0000068	Pa×s	998.17	Joback Method
dvisc	0.0000046	Pa×s	1094.53	Joback Method
dvisc	0.0000033	Pa×s	1190.89	Joback Method

Sources

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=C22432800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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