

Icosa-5,8,11,14-tetraenoic acid icosyl ester, Z,Z,Z,Z

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C40H72O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-42-40(

GVQSBNGRZGAXTP-NBORNWBVSA-N

C40H72O2

CCCCC=CCC=CCC=CCC=CCCCC(=O)OCCCCCCCCCCCCCCCCCCCCC

585.00

Physical Properties

Property code	Value	Unit	Source
gf	372.88	kJ/mol	Joback Method
hf	-644.85	kJ/mol	Joback Method
hfus	102.95	kJ/mol	Joback Method
hvap	113.62	kJ/mol	Joback Method
log10ws	-14.84		Crippen Method
logp	13.717		Crippen Method
mcvol	564.700	ml/mol	McGowan Method
pc	433.31	kPa	Joback Method
rinpol	4066.48		NIST Webbook
rinpol	4066.48		NIST Webbook
tb	1207.53	K	Joback Method
tc	1602.77	K	Joback Method
tf	592.40	K	Joback Method
vc	2.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2124.37	J/mol×K	1207.53	Joback Method
cpg	2346.41	J/mol×K	1536.89	Joback Method
cpg	2299.72	J/mol×K	1471.02	Joback Method
cpg	2255.18	J/mol×K	1405.15	Joback Method
cpg	2211.78	J/mol×K	1339.28	Joback Method
cpg	2168.52	J/mol×K	1273.40	Joback Method
cpg	2396.28	J/mol×K	1602.77	Joback Method
dvisc	0.0000020	Pa×s	1207.53	Joback Method

dvisc	0.0000028	Pa×s	1105.01	Joback Method
dvisc	0.0000042	Pa×s	1002.49	Joback Method
dvisc	0.0000069	Pa×s	899.96	Joback Method
dvisc	0.0000129	Pa×s	797.44	Joback Method
dvisc	0.0000289	Pa×s	694.92	Joback Method
dvisc	0.0000854	Pa×s	592.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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