

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

Inchi:	InChI=1S/C36H64O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-24-26-28-30-32-34-36(37)38-
InchiKey:	WDZUHOOLQVWVLI-DCSOTDLTSA-N
Formula:	C36H64O2
SMILES:	CCCCC=CCC=CCC=CCC=CCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	528.89

Physical Properties

Property code	Value	Unit	Source
gf	339.20	kJ/mol	Joback Method
hf	-562.29	kJ/mol	Joback Method
hfus	92.59	kJ/mol	Joback Method
hvap	104.72	kJ/mol	Joback Method
log10ws	-13.17		Crippen Method
logp	12.157		Crippen Method
mcvol	508.340	ml/mol	McGowan Method
pc	511.87	kPa	Joback Method
rinpol	3660.65		NIST Webbook
rinpol	3660.65		NIST Webbook
tb	1116.01	K	Joback Method
tc	1420.29	K	Joback Method
tf	547.32	K	Joback Method
vc	1.996	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1844.08	J/molxK	1116.01	Joback Method
cpg	1877.03	J/molxK	1166.72	Joback Method
cpg	1908.75	J/molxK	1217.44	Joback Method
cpg	1939.65	J/molxK	1268.15	Joback Method
cpg	1970.18	J/molxK	1318.87	Joback Method
cpg	2000.75	J/molxK	1369.58	Joback Method
cpg	2031.78	J/molxK	1420.29	Joback Method
dvisc	0.0001575	Paxs	547.32	Joback Method

dvisc	0.0000539	Paxs	642.10	Joback Method
dvisc	0.0000243	Paxs	736.88	Joback Method
dvisc	0.0000132	Paxs	831.66	Joback Method
dvisc	0.0000081	Paxs	926.45	Joback Method
dvisc	0.0000054	Paxs	1021.23	Joback Method
dvisc	0.0000039	Paxs	1116.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436732&Units=SI

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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