

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

Inchi:	InChI=1S/C34H60O2/c1-3-5-7-9-11-13-15-17-18-19-20-21-22-24-26-28-30-32-34(35)36-
InchiKey:	FWIBXYFQRWPVFD-KXGNKILUSA-N
Formula:	C34H60O2
SMILES:	CCCCC=CCC=CCC=CCC=CCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	500.84

Physical Properties

Property code	Value	Unit	Source
gf	322.36	kJ/mol	Joback Method
hf	-521.01	kJ/mol	Joback Method
hfus	87.41	kJ/mol	Joback Method
hvap	100.27	kJ/mol	Joback Method
log10ws	-12.33		Crippen Method
logp	11.376		Crippen Method
mcvol	480.160	ml/mol	McGowan Method
pc	559.41	kPa	Joback Method
rinpol	3459.60		NIST Webbook
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tb	1070.25	K	Joback Method
tc	1341.75	K	Joback Method
tf	524.78	K	Joback Method
vc	1.883	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1706.86	J/molxK	1070.25	Joback Method
cpg	1843.24	J/molxK	1296.50	Joback Method
cpg	1817.21	J/molxK	1251.25	Joback Method
cpg	1790.85	J/molxK	1206.00	Joback Method
cpg	1763.87	J/molxK	1160.75	Joback Method
cpg	1735.97	J/molxK	1115.50	Joback Method
cpg	1869.21	J/molxK	1341.75	Joback Method
dvisc	0.0000054	Paxs	1070.25	Joback Method

dvisc	0.0000074	Paxs	979.34	Joback Method
dvisc	0.0000111	Paxs	888.43	Joback Method
dvisc	0.0000180	Paxs	797.51	Joback Method
dvisc	0.0000331	Paxs	706.60	Joback Method
dvisc	0.0000730	Paxs	615.69	Joback Method
dvisc	0.0002118	Paxs	524.78	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=R436554&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

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