

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

Inchi:	InChI=1S/C38H68O2/c1-3-5-7-9-11-13-15-17-19-21-22-24-26-28-30-32-34-36-38(39)40-
InchiKey:	INCGCRQVVSKVJP-LGHBDAFPSA-N
Formula:	C38H68O2
SMILES:	CCCCC=CCC=CCC=CCC=CCCC(=O)OCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	556.95

Physical Properties

Property code	Value	Unit	Source
gf	356.04	kJ/mol	Joback Method
hf	-603.57	kJ/mol	Joback Method
hfus	97.77	kJ/mol	Joback Method
hvap	109.17	kJ/mol	Joback Method
log10ws	-14.01		Crippen Method
logp	12.937		Crippen Method
mcvol	536.520	ml/mol	McGowan Method
pc	470.13	kPa	Joback Method
rinpol	3863.07		NIST Webbook
rinpol	3863.07		NIST Webbook
tb	1161.77	K	Joback Method
tc	1506.82	K	Joback Method
tf	569.86	K	Joback Method
vc	2.107	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1983.26	J/molxK	1161.77	Joback Method
cpg	2167.38	J/molxK	1449.31	Joback Method
cpg	2130.29	J/molxK	1391.80	Joback Method
cpg	2093.99	J/molxK	1334.29	Joback Method
cpg	2057.81	J/molxK	1276.79	Joback Method
cpg	2021.12	J/molxK	1219.28	Joback Method
cpg	2205.89	J/molxK	1506.82	Joback Method
dvisc	0.0000028	Paxs	1161.77	Joback Method

dvisc	0.0000039	Paxs	1063.12	Joback Method
dvisc	0.0000059	Paxs	964.47	Joback Method
dvisc	0.0000096	Paxs	865.81	Joback Method
dvisc	0.0000178	Paxs	767.16	Joback Method
dvisc	0.0000396	Paxs	668.51	Joback Method
dvisc	0.0001163	Paxs	569.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R436910&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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