

Triarachine

Other names:

Triarachidin
Eicosanoic acid, 1,2,3-propanetriyl ester
Triaachidin
1,2,3-Propanetriol trieicosanoate
Propane-1,2,3-triyl triicosanoate
Glyceryl triarachidate
Glycerol triarachidate
Triarachidoylglycerol

Inchi:

InChI=1S/C63H122O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-52-55-61(64)

InchiKey:

KCVWRCXEUJUXIG-UHFFFAOYSA-N

Formula:

C63H122O6

SMILES:

CCCCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]:

975.64

CAS:

620-64-4

Physical Properties

Property code	Value	Unit	Source
chs	-39467.70 ± 1.80	kJ/mol	NIST Webbook
gf	-224.62	kJ/mol	Joback Method
hf	-2083.33	kJ/mol	Joback Method
hfus	163.76	kJ/mol	Joback Method
hvap	182.91	kJ/mol	Joback Method
log10ws	-22.89		Crippen Method
logp	21.110		Crippen Method
mcvol	920.850	ml/mol	McGowan Method
pc	197.26	kPa	Joback Method
tb	1869.27	K	Joback Method
tc	10477.66	K	Joback Method
tf	1001.25	K	Joback Method
tt	335.50 ± 1.00	K	NIST Webbook
tt	351.50 ± 1.00	K	NIST Webbook
tt	342.40 ± 1.00	K	NIST Webbook
vc	3.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3762.61	J/molxK	1869.27	Joback Method
cpg	5715.30	J/molxK	3304.00	Joback Method
cpg	17545.35	J/molxK	4738.73	Joback Method
cpg	48936.37	J/molxK	6173.47	Joback Method
cpg	109571.98	J/molxK	7608.20	Joback Method
cpg	209135.83	J/molxK	9042.93	Joback Method
cpg	357311.52	J/molxK	10477.66	Joback Method
dvisc	0.0000006	Paxs	1001.25	Joback Method
dvisc	0.0000003	Paxs	1145.92	Joback Method
dvisc	0.0000001	Paxs	1290.59	Joback Method
dvisc	6.8574290e-08	Paxs	1435.26	Joback Method
dvisc	4.2809272e-08	Paxs	1579.93	Joback Method
dvisc	2.8923078e-08	Paxs	1724.60	Joback Method
dvisc	2.0763975e-08	Paxs	1869.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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