

(Z)-(Z)-Tetracos-15-en-1-yl icos-11-enoate

Inchi:	InChI=1S/C44H84O2/c1-3-5-7-9-11-13-15-17-19-21-22-23-24-25-27-29-31-33-35-37-39-
InchiKey:	XMZFOULJKLPCFF-CLFAGFIQSA-N
Formula:	C44H84O2
SMILES:	CCCCCCCC=CCCCCCCCCCCCCCCCOC(=O)CCCCCCCC=CCCCCCCC
Mol. weight [g/mol]:	645.14
CAS:	872411-99-9

Physical Properties

Property code	Value	Unit	Source
gf	246.12	kJ/mol	Joback Method
hf	-961.85	kJ/mol	Joback Method
hfus	112.91	kJ/mol	Joback Method
hvap	122.61	kJ/mol	Joback Method
log10ws	-16.81		Crippen Method
logp	15.725		Crippen Method
mvol	629.660	ml/mol	McGowan Method
pc	357.08	kPa	Joback Method
rinpol	5763.90		NIST Webbook
rinpol	5763.90		NIST Webbook
tb	1290.73	K	Joback Method
tc	1861.65	K	Joback Method
tf	647.64	K	Joback Method
vc	2.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2458.73	J/molxK	1290.73	Joback Method
cpg	2749.63	J/molxK	1766.50	Joback Method
cpg	2685.60	J/molxK	1671.35	Joback Method
cpg	2627.30	J/molxK	1576.19	Joback Method
cpg	2571.93	J/molxK	1481.04	Joback Method
cpg	2516.67	J/molxK	1385.88	Joback Method
cpg	2822.21	J/molxK	1861.65	Joback Method

dvisc	0.0000013	Paxs	1290.73	Joback Method
dvisc	0.0000018	Paxs	1183.55	Joback Method
dvisc	0.0000028	Paxs	1076.37	Joback Method
dvisc	0.0000045	Paxs	969.18	Joback Method
dvisc	0.0000083	Paxs	862.00	Joback Method
dvisc	0.0000182	Paxs	754.82	Joback Method
dvisc	0.0000519	Paxs	647.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C872411999&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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