

(Z)-1,3-Dimethoxypropan-2-yl icos-11-enoate

Inchi:	InChI=1S/C25H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25(26)29-24
InchiKey:	ZKIVTPVYCIAXCY-QXMHVHEDSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCC=CCCCCCCCCCC(=O)OC(COC)COC
Mol. weight [g/mol]:	412.65

Physical Properties

Property code	Value	Unit	Source
gf	-206.52	kJ/mol	Joback Method
hf	-956.63	kJ/mol	Joback Method
hfus	62.35	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	7.009		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	896.25	K	Joback Method
tc	1098.52	K	Joback Method
tf	468.05	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.72	J/molxK	896.25	Joback Method
cpg	1355.06	J/molxK	1064.81	Joback Method
cpg	1339.29	J/molxK	1031.10	Joback Method
cpg	1322.21	J/molxK	997.39	Joback Method
cpg	1303.77	J/molxK	963.67	Joback Method
cpg	1283.96	J/molxK	929.96	Joback Method
cpg	1369.55	J/molxK	1098.52	Joback Method
dvisc	0.0000159	Paxs	896.25	Joback Method

dvisc	0.0000218	Paxs	824.88	Joback Method
dvisc	0.0000318	Paxs	753.52	Joback Method
dvisc	0.0000502	Paxs	682.15	Joback Method
dvisc	0.0000883	Paxs	610.78	Joback Method
dvisc	0.0001800	Paxs	539.42	Joback Method
dvisc	0.0004564	Paxs	468.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412821&Units=SI
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

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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