

METHYL (11R,12R,13S)-(Z)-12,13-EPOXY-11-METHOXY-9-O

Other names: Methyl (Z)-12,13-epoxy-11-methoxy-9-octadecenoate

Inchi: InChI=1S/C20H36O4/c1-4-5-11-15-18-20(24-18)17(22-2)14-12-9-7-6-8-10-13-16-19(21)2

InchiKey: BOCZHGZTZHPCHP-WYMLVPIESA-N

Formula: C20H36O4

SMILES: CCCCCC1OC1C(/C=C/CCCCCCCC(=O)OC)OC

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
hf	-841.77	kJ/mol	Cheméo Relay (1.0)
hfus	55.40	kJ/mol	Joback Method
hvap	107.04	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.71		Cheméo Relay (1.0)
logp	4.809		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
rinpol	2521.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	610.68	K	Cheméo Relay (1.0)
tc	799.91	K	Cheméo Relay (1.0)
tf	322.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.48	J/mol×K	788.45	Joback Method
cpg	1041.57	J/mol×K	973.76	Joback Method
cpg	1027.31	J/mol×K	942.87	Joback Method
cpg	1012.20	J/mol×K	911.99	Joback Method
cpg	996.20	J/mol×K	881.10	Joback Method
cpg	979.28	J/mol×K	850.22	Joback Method
cpg	961.38	J/mol×K	819.33	Joback Method
dvisc	0.0003226	Pa×s	609.10	Joback Method
dvisc	0.0001439	Pa×s	788.45	Joback Method

dvisc	0.0001802	Pa×s	728.66	Joback Method
dvisc	0.0002349	Pa×s	668.88	Joback Method
dvisc	0.0014187	Pa×s	429.74	Joback Method
dvisc	0.0004747	Pa×s	549.31	Joback Method
dvisc	0.0007676	Pa×s	489.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88335391&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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