

9,12-Octadecadienal, dimethyl acetal

Inchi:	InChI=1S/C20H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21-2)22-3/h8-9,
InchiKey:	AEIAXQVKYHJVFA-MVKOLZDDSA-N
Formula:	C20H38O2
SMILES:	CCCCC=CCC=CCCCCCCCC(OC)OC
Mol. weight [g/mol]:	310.51
CAS:	1599-51-5

Physical Properties

Property code	Value	Unit	Source
gf	65.52	kJ/mol	Joback Method
hf	-491.41	kJ/mol	Joback Method
hfus	46.81	kJ/mol	Joback Method
hvap	64.46	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.419		Crippen Method
mvol	295.800	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	2422.00		NIST Webbook
tb	709.72	K	Joback Method
tc	882.40	K	Joback Method
tf	334.46	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.10	J/molxK	709.72	Joback Method
cpg	884.93	J/molxK	738.50	Joback Method
cpg	903.85	J/molxK	767.28	Joback Method
cpg	921.91	J/molxK	796.06	Joback Method
cpg	939.13	J/molxK	824.84	Joback Method
cpg	955.53	J/molxK	853.62	Joback Method
cpg	971.16	J/molxK	882.40	Joback Method
dvisc	0.0018328	Paxs	334.46	Joback Method

dvisc	0.0005840	Paxs	397.00	Joback Method
dvisc	0.0002540	Paxs	459.55	Joback Method
dvisc	0.0001349	Paxs	522.09	Joback Method
dvisc	0.0000820	Paxs	584.63	Joback Method
dvisc	0.0000549	Paxs	647.18	Joback Method
dvisc	0.0000394	Paxs	709.72	Joback Method

Sources

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=C1599515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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