7,7-Dimethyl-(5Z,8Z)-eicosadienoic acid, methyl ester

Inchi: InChI=1S/C23H42O2/c1-5-6-7-8-9-10-11-12-13-14-17-20-23(2,3)21-18-15-16-19-22(24)2

InchiKey: REOUXWGNXBUTOE-HIOQQWDOSA-N

Formula: C23H42O2

SMILES: CCCCCCCCCCCC=CC(C)(C)C=CCCCC(=O)OC

Mol. weight [g/mol]: 350.58

Physical Properties

Property code	Value	Unit	Source
gf	72.14	kJ/mol	Joback Method
hf	-537.16	kJ/mol	Joback Method
hfus	51.10	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	7.389		Crippen Method
mcvol	333.770	ml/mol	McGowan Method
pc	942.68	kPa	Joback Method
rinpol	2365.20		NIST Webbook
rinpol	2365.20		NIST Webbook
tb	807.02	K	Joback Method
tc	993.53	K	Joback Method
tf	413.39	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.75	J/mol×K	807.02	Joback Method
cpg	1064.68	J/mol×K	838.10	Joback Method
cpg	1083.60	J/mol×K	869.19	Joback Method
cpg	1101.59	J/mol×K	900.27	Joback Method
cpg	1118.70	J/mol×K	931.36	Joback Method
cpg	1135.01	J/mol×K	962.44	Joback Method
cpg	1150.59	J/mol×K	993.53	Joback Method
dvisc	0.0010544	Pa×s	413.39	Joback Method

dvisc	0.0003854	Pa×s	479.00	Joback Method
dvisc	0.0001796	Pa×s	544.60	Joback Method
dvisc	0.0000986	Pa×s	610.21	Joback Method
dvisc	0.0000608	Pa×s	675.81	Joback Method
dvisc	0.0000409	Pa×s	741.41	Joback Method
dvisc	0.0000293	Pa×s	807.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333537&Units=SI
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

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