10,12-Tricosadiynoic acid, methyl ester

Inchi: InChI=1S/C24H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24(2
InchiKey: BZHUUTOAKXXTMA-UHFFFAOYSA-N
Formula: C24H40O2
SMILES: CCCCCCCCCCC#CC#CCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 360.57

Physical Properties

Property code	Value	Unit	Source
gf	322.88	kJ/mol	Joback Method
hf	-238.89	kJ/mol	Joback Method
hfus	66.95	kJ/mol	Joback Method
hvap	82.48	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	6.818		Crippen Method
mcvol	339.260	ml/mol	McGowan Method
pc	1003.98	kPa	Joback Method
rinpol	2832.30		NIST Webbook
rinpol	2832.30		NIST Webbook
tb	842.81	K	Joback Method
tc	1038.10	K	Joback Method
tf	644.60	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.94	J/mol×K	842.81	Joback Method
cpg	1077.58	J/mol×K	875.36	Joback Method
cpg	1096.10	J/mol×K	907.91	Joback Method
cpg	1113.55	J/mol×K	940.45	Joback Method
cpg	1129.95	J/mol×K	973.00	Joback Method
cpg	1145.34	J/mol×K	1005.55	Joback Method
cpg	1159.76	J/mol×K	1038.10	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=U333594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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