5,8,11-Eicosatriynoic acid, methyl ester

Inchi: InChI=1S/C21H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h3
InchiKey: KMJIYNMTPBHYPF-UHFFFAOYSA-N
Formula: C21H30O2
SMILES: CCCCCCCCC#CCC#CCC#CCCCC(=O)OC
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	500.42	kJ/mol	Joback Method
hf	95.33	kJ/mol	Joback Method
hfus	62.30	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	4.871		Crippen Method
mcvol	288.390	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	2465.10		NIST Webbook
tb	783.17	K	Joback Method
tc	990.12	K	Joback Method
tf	716.89	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.08	J/mol×K	783.17	Joback Method
cpg	846.45	J/mol×K	817.66	Joback Method
cpg	863.78	J/mol×K	852.15	Joback Method
cpg	880.09	J/mol×K	886.65	Joback Method
cpg	895.42	J/mol×K	921.14	Joback Method
cpg	909.78	J/mol×K	955.63	Joback Method
cpg	923.21	J/mol×K	990.12	Joback Method

Sources

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=U333561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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