5,8,11,14-Eicosatetraynoic acid, methyl ester

Inchi: InChI=1S/C21H26O2/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: CTHYLKQCJHFQOG-UHFFFAOYSA-N
Formula: C21H26O2
SMILES: CCCCCC#CCC#CCC#CCC#CCCCC(=O)OC
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	703.22	kJ/mol	Joback Method
hf	367.63	kJ/mol	Joback Method
hfus	65.42	kJ/mol	Joback Method
hvap	80.10	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	4.094		Crippen Method
mcvol	279.790	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook
tb	792.17	K	Joback Method
tc	1016.94	K	Joback Method
tf	822.99	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.24	J/mol×K	792.17	Joback Method
cpg	797.28	J/mol×K	829.63	Joback Method
cpg	814.21	J/mol×K	867.09	Joback Method
cpg	830.06	J/mol×K	904.55	Joback Method
cpg	844.86	J/mol×K	942.02	Joback Method
cpg	858.64	J/mol×K	979.48	Joback Method
cpg	871.43	J/mol×K	1016.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333545&Units=SI

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