Methyl 3,7,11,15-tetramethylhexadec-2-enoate

Inchi: InChI=1S/C21H40O2/c1-17(2)10-7-11-18(3)12-8-13-19(4)14-9-15-20(5)16-21(22)23-6/h1
InchiKey: WISPDDYDWJMVMK-CAPFRKAQSA-N
Formula: C21H40O2
SMILES: COC(=O)C=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 324.54
CAS: 64433-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-43.63	kJ/mol	Joback Method
hf	-629.98	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	70.37	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.545		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	2185.80		NIST Webbook
rinpol	2185.80		NIST Webbook
tb	758.89	K	Joback Method
tc	940.42	K	Joback Method
tf	334.55	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.66	J/mol×K	758.89	Joback Method
cpg	966.82	J/mol×K	789.15	Joback Method
cpg	985.96	J/mol×K	819.40	Joback Method
cpg	1004.12	J/mol×K	849.66	Joback Method
cpg	1021.33	J/mol×K	879.91	Joback Method
cpg	1037.63	J/mol×K	910.17	Joback Method
cpg	1053.05	J/mol×K	940.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64433358&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
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