Undec-10-ynoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C19H32O2/c1-4-6-8-10-11-12-13-15-17-19(20)21-18(3)16-14-9-7-5-2/h1,14,16
InchiKey: FNRWYESTOQNFSD-JQIJEIRASA-N
Formula: C19H32O2
SMILES: C#CCCCCCCCCC(=O)OC(C)C=CCCCC
Mol. weight [g/mol]: 292.46

Physical Properties

Property code	Value	Unit	Source
gf	176.03	kJ/mol	Joback Method
hf	-276.45	kJ/mol	Joback Method
hfus	47.41	kJ/mol	Joback Method
hvap	66.47	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.418		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	704.25	K	Joback Method
tc	884.88	K	Joback Method
tf	402.94	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.09	J/mol×K	704.25	Joback Method
cpg	794.15	J/mol×K	734.36	Joback Method
cpg	811.34	J/mol×K	764.46	Joback Method
cpg	827.67	J/mol×K	794.57	Joback Method
cpg	843.20	J/mol×K	824.67	Joback Method
cpg	857.95	J/mol×K	854.78	Joback Method
cpg	871.96	J/mol×K	884.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406965&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

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