Undec-10-ynoic acid, 4-methyl-2-pentyl ester

Inchi: InChI=1S/C17H30O2/c1-5-6-7-8-9-10-11-12-13-17(18)19-16(4)14-15(2)3/h1,15-16H,6-14
InchiKey: BYXWOWQRJAMVFW-UHFFFAOYSA-N
Formula: C17H30O2
SMILES: C#CCCCCCCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	76.53	kJ/mol	Joback Method
hf	-357.67	kJ/mol	Joback Method
hfus	38.50	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.718		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
tb	653.89	K	Joback Method
tc	832.78	K	Joback Method
tf	370.48	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.61	J/mol×K	653.89	Joback Method
cpg	703.64	J/mol×K	683.70	Joback Method
cpg	720.83	J/mol×K	713.52	Joback Method
cpg	737.19	J/mol×K	743.33	Joback Method
cpg	752.75	J/mol×K	773.15	Joback Method
cpg	767.53	J/mol×K	802.96	Joback Method
cpg	781.55	J/mol×K	832.78	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=U406158&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