Undec-10-ynoic acid, hexyl ester

Inchi: InChI=1S/C17H30O2/c1-3-5-7-9-10-11-12-13-15-17(18)19-16-14-8-6-4-2/h1H,4-16H2,2H
InchiKey: RGECZIIDDYVYOB-UHFFFAOYSA-N
Formula: C17H30O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	81.41	kJ/mol	Joback Method
hf	-347.11	kJ/mol	Joback Method
hfus	45.55	kJ/mol	Joback Method
hvap	62.45	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.864		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
tb	654.77	K	Joback Method
tc	828.64	K	Joback Method
tf	400.48	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.79	J/mol×K	654.77	Joback Method
cpg	702.25	J/mol×K	683.75	Joback Method
cpg	718.92	J/mol×K	712.73	Joback Method
cpg	734.83	J/mol×K	741.71	Joback Method
cpg	749.99	J/mol×K	770.68	Joback Method
cpg	764.43	J/mol×K	799.66	Joback Method
cpg	778.17	J/mol×K	828.64	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=U406159&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