Undec-10-ynoic acid, heptyl ester

Inchi: InChI=1S/C18H32O2/c1-3-5-7-9-10-11-12-14-16-18(19)20-17-15-13-8-6-4-2/h1H,4-17H2
InchiKey: MKFIZUJFXMISMS-UHFFFAOYSA-N
Formula: C18H32O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 280.45

Physical Properties

Property code	Value	Unit	Source
gf	89.83	kJ/mol	Joback Method
hf	-367.75	kJ/mol	Joback Method
hfus	48.14	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.254		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	677.65	K	Joback Method
tc	851.34	K	Joback Method
tf	411.75	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.83	J/mol×K	677.65	Joback Method
cpg	758.71	J/mol×K	706.60	Joback Method
cpg	775.78	J/mol×K	735.55	Joback Method
cpg	792.05	J/mol×K	764.49	Joback Method
cpg	807.55	J/mol×K	793.44	Joback Method
cpg	822.31	J/mol×K	822.39	Joback Method
cpg	836.34	J/mol×K	851.34	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=U406160&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

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