Undec-10-ynoic acid, pentyl ester

Inchi: InChI=1S/C16H28O2/c1-3-5-7-8-9-10-11-12-14-16(17)18-15-13-6-4-2/h1H,4-15H2,2H3
InchiKey: HFRFJCGGYQZDME-UHFFFAOYSA-N
Formula: C16H28O2
SMILES: C#CCCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	72.99	kJ/mol	Joback Method
hf	-326.47	kJ/mol	Joback Method
hfus	42.96	kJ/mol	Joback Method
hvap	60.22	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.474		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	631.89	K	Joback Method
tc	806.35	K	Joback Method
tf	389.21	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.03	J/mol×K	631.89	Joback Method
cpg	647.03	J/mol×K	660.97	Joback Method
cpg	663.28	J/mol×K	690.04	Joback Method
cpg	678.79	J/mol×K	719.12	Joback Method
cpg	693.59	J/mol×K	748.19	Joback Method
cpg	707.68	J/mol×K	777.27	Joback Method
cpg	721.10	J/mol×K	806.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406166&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