Undec-10-ynoic acid, heptadecyl ester

Inchi: InChI=1S/C28H52O2/c1-3-5-7-9-11-13-14-15-16-17-18-19-21-23-25-27-30-28(29)26-24-
InchiKey: UCTUWLQBNDCKIQ-UHFFFAOYSA-N
Formula: C28H52O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 420.71

Physical Properties

Property code	Value	Unit	Source
gf	174.03	kJ/mol	Joback Method
hf	-574.15	kJ/mol	Joback Method
hfus	74.04	kJ/mol	Joback Method
hvap	86.94	kJ/mol	Joback Method
log10ws	-10.20		Crippen Method
logp	9.155		Crippen Method
mcvol	404.220	ml/mol	McGowan Method
pc	725.75	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	906.45	K	Joback Method
tc	1112.47	K	Joback Method
tf	524.45	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.81	J/mol×K	906.45	Joback Method
cpg	1377.60	J/mol×K	940.79	Joback Method
cpg	1399.02	J/mol×K	975.12	Joback Method
cpg	1419.13	J/mol×K	1009.46	Joback Method
cpg	1437.98	J/mol×K	1043.80	Joback Method
cpg	1455.67	J/mol×K	1078.13	Joback Method
cpg	1472.24	J/mol×K	1112.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406170&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