Undec-10-ynoic acid, octadecyl ester

Inchi: InChI=1S/C29H54O2/c1-3-5-7-9-11-13-14-15-16-17-18-19-20-22-24-26-28-31-29(30)27-
InchiKey: GIXXCJBLAKJFIX-UHFFFAOYSA-N
Formula: C29H54O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 434.74

Physical Properties

Property code	Value	Unit	Source
gf	182.45	kJ/mol	Joback Method
hf	-594.79	kJ/mol	Joback Method
hfus	76.63	kJ/mol	Joback Method
hvap	89.16	kJ/mol	Joback Method
log10ws	-10.62		Crippen Method
logp	9.545		Crippen Method
mcvol	418.310	ml/mol	McGowan Method
pc	689.61	kPa	Joback Method
rinpol	3007.00		NIST Webbook
rinpol	3007.00		NIST Webbook
tb	929.33	K	Joback Method
tc	1143.42	K	Joback Method
tf	535.72	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1420.10	J/mol×K	929.33	Joback Method
cpg	1443.66	J/mol×K	965.01	Joback Method
cpg	1465.72	J/mol×K	1000.69	Joback Method
cpg	1486.37	J/mol×K	1036.38	Joback Method
cpg	1505.70	J/mol×K	1072.06	Joback Method
cpg	1523.76	J/mol×K	1107.74	Joback Method
cpg	1540.66	J/mol×K	1143.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406171&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