Undec-10-ynoic acid, hexadecyl ester

Inchi: InChI=1S/C27H50O2/c1-3-5-7-9-11-13-14-15-16-17-18-20-22-24-26-29-27(28)25-23-21-
InchiKey: AHAMRTRAKUNZMP-UHFFFAOYSA-N
Formula: C27H50O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 406.68

Physical Properties

Property code	Value	Unit	Source
gf	165.61	kJ/mol	Joback Method
hf	-553.51	kJ/mol	Joback Method
hfus	71.45	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.765		Crippen Method
mcvol	390.130	ml/mol	McGowan Method
pc	764.79	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook
tb	883.57	K	Joback Method
tc	1082.62	K	Joback Method
tf	513.18	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.05	J/mol×K	883.57	Joback Method
cpg	1312.16	J/mol×K	916.74	Joback Method
cpg	1332.99	J/mol×K	949.92	Joback Method
cpg	1352.59	J/mol×K	983.09	Joback Method
cpg	1371.02	J/mol×K	1016.27	Joback Method
cpg	1388.34	J/mol×K	1049.44	Joback Method
cpg	1404.61	J/mol×K	1082.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406169&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