Undec-10-ynoic acid, pentadecyl ester

Inchi: InChI=1S/C26H48O2/c1-3-5-7-9-11-13-14-15-16-17-19-21-23-25-28-26(27)24-22-20-18-
InchiKey: UYXZZLUOPYJUTI-UHFFFAOYSA-N
Formula: C26H48O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 392.66

Physical Properties

Property code	Value	Unit	Source
gf	157.19	kJ/mol	Joback Method
hf	-532.87	kJ/mol	Joback Method
hfus	68.86	kJ/mol	Joback Method
hvap	82.48	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	8.375		Crippen Method
mcvol	376.040	ml/mol	McGowan Method
pc	807.08	kPa	Joback Method
rinpol	2712.00		NIST Webbook
rinpol	2712.00		NIST Webbook
tb	860.69	K	Joback Method
tc	1053.79	K	Joback Method
tf	501.91	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.88	J/mol×K	860.69	Joback Method
cpg	1247.37	J/mol×K	892.87	Joback Method
cpg	1267.66	J/mol×K	925.06	Joback Method
cpg	1286.80	J/mol×K	957.24	Joback Method
cpg	1304.83	J/mol×K	989.42	Joback Method
cpg	1321.82	J/mol×K	1021.60	Joback Method
cpg	1337.81	J/mol×K	1053.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406168&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