Undec-10-ynoic acid, undec-2-en-1-yl ester

Inchi: InChI=1S/C22H38O2/c1-3-5-7-9-11-13-15-17-19-21-24-22(23)20-18-16-14-12-10-8-6-4-2
InchiKey: VMWNNSMMRDOOQX-HTXNQAPBSA-N
Formula: C22H38O2
SMILES: C#CCCCCCCCCC(=O)OCC=CCCCCCCCC
Mol. weight [g/mol]: 334.54

Physical Properties

Property code	Value	Unit	Source
gf	203.73	kJ/mol	Joback Method
hf	-333.09	kJ/mol	Joback Method
hfus	58.70	kJ/mol	Joback Method
hvap	73.54	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.590		Crippen Method
mcvol	315.380	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2406.00		NIST Webbook
rinpol	2406.00		NIST Webbook
tb	773.33	K	Joback Method
tc	954.38	K	Joback Method
tf	451.75	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.07	J/mol×K	773.33	Joback Method
cpg	971.04	J/mol×K	803.51	Joback Method
cpg	989.08	J/mol×K	833.68	Joback Method
cpg	1006.23	J/mol×K	863.86	Joback Method
cpg	1022.52	J/mol×K	894.03	Joback Method
cpg	1038.00	J/mol×K	924.21	Joback Method
cpg	1052.72	J/mol×K	954.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406968&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