Undec-10-ynoic acid, undecyl ester

Inchi: InChI=1S/C22H40O2/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: WJDYXMOOBBAZOX-UHFFFAOYSA-N
Formula: C22H40O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 336.55

Physical Properties

Property code	Value	Unit	Source
gf	123.51	kJ/mol	Joback Method
hf	-450.31	kJ/mol	Joback Method
hfus	58.50	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.814		Crippen Method
mcvol	319.680	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2308.00		NIST Webbook
tb	769.17	K	Joback Method
tc	947.15	K	Joback Method
tf	456.83	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.18	J/mol×K	769.17	Joback Method
cpg	995.69	J/mol×K	798.83	Joback Method
cpg	1014.23	J/mol×K	828.50	Joback Method
cpg	1031.84	J/mol×K	858.16	Joback Method
cpg	1048.55	J/mol×K	887.83	Joback Method
cpg	1064.39	J/mol×K	917.49	Joback Method
cpg	1079.40	J/mol×K	947.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406164&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