Undec-10-ynoic acid, decyl ester

Inchi: InChI=1S/C21H38O2/c1-3-5-7-9-11-13-15-17-19-21(22)23-20-18-16-14-12-10-8-6-4-2/h1
InchiKey: WIBJHNGPNUHEMK-UHFFFAOYSA-N
Formula: C21H38O2
SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 322.53

Physical Properties

Property code	Value	Unit	Source
gf	115.09	kJ/mol	Joback Method
hf	-429.67	kJ/mol	Joback Method
hfus	55.91	kJ/mol	Joback Method
hvap	71.35	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.424		Crippen Method
mcvol	305.590	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	746.29	K	Joback Method
tc	922.33	K	Joback Method
tf	445.56	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.82	J/mol×K	746.29	Joback Method
cpg	934.91	J/mol×K	775.63	Joback Method
cpg	953.08	J/mol×K	804.97	Joback Method
cpg	970.36	J/mol×K	834.31	Joback Method
cpg	986.77	J/mol×K	863.65	Joback Method
cpg	1002.35	J/mol×K	892.99	Joback Method
cpg	1017.13	J/mol×K	922.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406163&Units=SI

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