Undec-10-ynoic acid, nonyl ester

Inchi: InChI=1S/C20H36O2/c1-3-5-7-9-11-12-14-16-18-20(21)22-19-17-15-13-10-8-6-4-2/h1H,4

InchiKey: XLFKMHBUVLALDA-UHFFFAOYSA-N

Formula: C20H36O2

SMILES: C#CCCCCCCCCC(=O)OCCCCCCCCC

Mol. weight [g/mol]: 308.50

Physical Properties

Property code	Value	Unit	Source
gf	106.67	kJ/mol	Joback Method
hf	-409.03	kJ/mol	Joback Method
hfus	53.32	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.034		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	723.41	K	Joback Method
tc	898.13	K	Joback Method
tf	434.29	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.43	J/mol×K	723.41	Joback Method
cpg	875.11	J/mol×K	752.53	Joback Method
cpg	892.92	J/mol×K	781.65	Joback Method
cpg	909.87	J/mol×K	810.77	Joback Method
cpg	925.99	J/mol×K	839.89	Joback Method
cpg	941.30	J/mol×K	869.01	Joback Method
cpg	955.84	J/mol×K	898.13	Joback Method

Sources

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=U406162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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