Octanoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C21H38O2/c1-3-5-7-9-10-11-12-13-14-16-18-20-23-21(22)19-17-15-8-6-4-2/h3
InchiKey: GHCSOROVZMLBDG-UHFFFAOYSA-N
Formula: C21H38O2
SMILES: CCCCCCCCCCC#CCOC(=O)CCCCCCC
Mol. weight [g/mol]: 322.53

Physical Properties

Property code	Value	Unit	Source
gf	94.82	kJ/mol	Joback Method
hf	-449.27	kJ/mol	Joback Method
hfus	56.05	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.424		Crippen Method
mcvol	305.590	ml/mol	McGowan Method
pc	1090.66	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	765.17	K	Joback Method
tc	946.83	K	Joback Method
tf	504.69	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.14	J/mol×K	765.17	Joback Method
cpg	942.50	J/mol×K	795.45	Joback Method
cpg	960.89	J/mol×K	825.72	Joback Method
cpg	978.33	J/mol×K	856.00	Joback Method
cpg	994.85	J/mol×K	886.28	Joback Method
cpg	1010.48	J/mol×K	916.55	Joback Method
cpg	1025.24	J/mol×K	946.83	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=U299349&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