Oct-3-enoic acid, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C21H36O2/c1-3-5-7-9-10-11-12-13-14-16-18-20-23-21(22)19-17-15-8-6-4-2/h1
InchiKey: GBPNNTPKVDQNPK-BMRADRMJSA-N
Formula: C21H36O2
SMILES: CCCCC=CCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]: 320.51

Physical Properties

Property code	Value	Unit	Source
gf	175.04	kJ/mol	Joback Method
hf	-332.05	kJ/mol	Joback Method
hfus	56.26	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.200		Crippen Method
mcvol	301.290	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	769.33	K	Joback Method
tc	954.79	K	Joback Method
tf	499.61	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.05	J/mol×K	769.33	Joback Method
cpg	917.93	J/mol×K	800.24	Joback Method
cpg	935.85	J/mol×K	831.15	Joback Method
cpg	952.86	J/mol×K	862.06	Joback Method
cpg	968.99	J/mol×K	892.97	Joback Method
cpg	984.28	J/mol×K	923.88	Joback Method
cpg	998.76	J/mol×K	954.79	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=U406954&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