Hexanoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C19H34O2/c1-3-5-7-8-9-10-11-12-13-14-16-18-21-19(20)17-15-6-4-2/h3-13,15
InchiKey: CZOVRBWHUCOPCC-UHFFFAOYSA-N
Formula: C19H34O2
SMILES: CCCCCCCCCCC#CCOC(=O)CCCCC
Mol. weight [g/mol]: 294.47

Physical Properties

Property code	Value	Unit	Source
gf	77.98	kJ/mol	Joback Method
hf	-407.99	kJ/mol	Joback Method
hfus	50.87	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.644		Crippen Method
mcvol	277.410	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	2082.00		NIST Webbook
tb	719.41	K	Joback Method
tc	899.63	K	Joback Method
tf	482.15	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.56	J/mol×K	719.41	Joback Method
cpg	823.21	J/mol×K	749.45	Joback Method
cpg	840.97	J/mol×K	779.48	Joback Method
cpg	857.85	J/mol×K	809.52	Joback Method
cpg	873.88	J/mol×K	839.56	Joback Method
cpg	889.08	J/mol×K	869.59	Joback Method
cpg	903.47	J/mol×K	899.63	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=U299360&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