Hexanoic acid, 3,5,5-trimethyl-, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C22H40O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-24-21(23)18-20(2)19-22(3,4)5

InchiKey: OYXBAGBKRSEBOW-UHFFFAOYSA-N

Formula: C22H40O2

SMILES: CCCCCCCCCCC#CCOC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 336.55

Physical Properties

Property code	Value	Unit	Source
gf	103.64	kJ/mol	Joback Method
hf	-483.94	kJ/mol	Joback Method
hfus	47.71	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.526		Crippen Method
mcvol	319.680	ml/mol	McGowan Method
pc	1042.60	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	784.38	K	Joback Method
tc	973.01	K	Joback Method
tf	503.38	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.40	J/mol×K	784.38	Joback Method
cpg	1005.46	J/mol×K	815.82	Joback Method
cpg	1024.44	J/mol×K	847.26	Joback Method
cpg	1042.38	J/mol×K	878.70	Joback Method
cpg	1059.34	J/mol×K	910.14	Joback Method
cpg	1075.35	J/mol×K	941.57	Joback Method
cpg	1090.45	J/mol×K	973.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406830&Units=SI
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

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