2-Heptenoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H26O2/c1-5-7-9-10-12-16(17)18-15(11-8-6-2)13-14(3)4/h10,12,14-15H,5-7
InchiKey: PKSRBOICWULCPD-ZRDIBKRKSA-N
Formula: C16H26O2
SMILES: CCC#CC(CC(C)C)OC(=O)C=CCCCC
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	128.06	kJ/mol	Joback Method
hf	-239.41	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	61.70	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.104		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
tb	654.05	K	Joback Method
tc	848.40	K	Joback Method
tf	413.26	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.61	J/mol×K	654.05	Joback Method
cpg	632.30	J/mol×K	686.44	Joback Method
cpg	649.09	J/mol×K	718.83	Joback Method
cpg	665.02	J/mol×K	751.22	Joback Method
cpg	680.12	J/mol×K	783.61	Joback Method
cpg	694.41	J/mol×K	816.01	Joback Method
cpg	707.92	J/mol×K	848.40	Joback Method

Sources

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=U406943&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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