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

Inchi: InChI=1S/C17H30O2/c1-5-7-9-10-11-13-17(18)19-16(12-8-6-2)14-15(3)4/h15-16H,5-7,9-
InchiKey: UYHUFAFUDXIGDI-UHFFFAOYSA-N
Formula: C17H30O2
SMILES: CCC#CC(CC(C)C)OC(=O)CCCCCCC
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	56.26	kJ/mol	Joback Method
hf	-377.27	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.718		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1710.00		NIST Webbook
tb	672.77	K	Joback Method
tc	858.99	K	Joback Method
tf	429.61	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.17	J/mol×K	672.77	Joback Method
cpg	709.66	J/mol×K	703.81	Joback Method
cpg	727.25	J/mol×K	734.84	Joback Method
cpg	743.97	J/mol×K	765.88	Joback Method
cpg	759.83	J/mol×K	796.92	Joback Method
cpg	774.85	J/mol×K	827.96	Joback Method
cpg	789.06	J/mol×K	858.99	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=U299345&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

Latest version available from:
https://www.chemeo.com/cid/58-005-2/Octanoic-acid-2-methyloct-5-yn-4-yl-ester.pdf
Generated by Cheméo on 2024-05-13 14:06:31.852438986 +0000 UTC m=+17898440.773016305.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.