Undec-10-ynoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C15H22O2/c1-4-6-7-8-9-10-11-12-13-15(16)17-14(3)5-2/h1-2,14H,6-13H2,3H3
InchiKey: WZSNKPVAHBCPQT-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C#CCCCCCCCCC(=O)OC(C)C#C
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	285.20	kJ/mol	Joback Method
hf	-19.21	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.305		Crippen Method
mcvol	212.450	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	598.69	K	Joback Method
tc	786.89	K	Joback Method
tf	409.91	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.20	J/mol×K	598.69	Joback Method
cpg	550.08	J/mol×K	630.06	Joback Method
cpg	565.17	J/mol×K	661.42	Joback Method
cpg	579.52	J/mol×K	692.79	Joback Method
cpg	593.15	J/mol×K	724.16	Joback Method
cpg	606.08	J/mol×K	755.53	Joback Method
cpg	618.34	J/mol×K	786.89	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=U406962&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