3-Methyl-2-butenoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C18H30O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-20-18(19)16-17(2)3/h16H,4-12,1
InchiKey: VKDYHHDVGVKPJS-UHFFFAOYSA-N
Formula: C18H30O2
SMILES: CCCCCCCCCCC#CCOC(=O)C=C(C)C
Mol. weight [g/mol]: 278.43

Physical Properties

Property code	Value	Unit	Source
gf	141.23	kJ/mol	Joback Method
hf	-279.92	kJ/mol	Joback Method
hfus	47.18	kJ/mol	Joback Method
hvap	67.01	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.030		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2035.00		NIST Webbook
tb	700.57	K	Joback Method
tc	888.32	K	Joback Method
tf	451.84	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.10	J/mol×K	700.57	Joback Method
cpg	742.13	J/mol×K	731.86	Joback Method
cpg	759.28	J/mol×K	763.15	Joback Method
cpg	775.57	J/mol×K	794.44	Joback Method
cpg	791.03	J/mol×K	825.73	Joback Method
cpg	805.71	J/mol×K	857.03	Joback Method
cpg	819.62	J/mol×K	888.32	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=U299317&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