Undec-10-ynoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C20H32O2/c1-5-7-9-10-11-12-13-14-16-20(21)22-19(15-8-6-2)17-18(3)4/h1,18

InchiKey: VWPUMBYYXCXPPZ-UHFFFAOYSA-N

Formula: C20H32O2

SMILES: C#CCCCCCCCCC(=O)OC(C#CCC)CC(C)C

Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	304.59	kJ/mol	Joback Method
hf	-147.29	kJ/mol	Joback Method
hfus	49.39	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.112		Crippen Method
mcvol	282.900	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	731.53	K	Joback Method
tc	922.70	K	Joback Method
tf	510.39	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.26	J/mol×K	731.53	Joback Method
cpg	830.90	J/mol×K	763.39	Joback Method
cpg	848.57	J/mol×K	795.25	Joback Method
cpg	865.30	J/mol×K	827.12	Joback Method
cpg	881.11	J/mol×K	858.98	Joback Method
cpg	896.04	J/mol×K	890.84	Joback Method
cpg	910.12	J/mol×K	922.70	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=U406966&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

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