Non-2-ynoic acid propyl ester

Inchi: InChI=1S/C12H20O2/c1-3-5-6-7-8-9-10-12(13)14-11-4-2/h3-8,11H2,1-2H3
InchiKey: FSXFHENNXHPKBA-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CCCCCCC#CC(=O)OCCC
Mol. weight [g/mol]: 196.29
CAS: 15860-54-5

Physical Properties

Property code	Value	Unit	Source
gf	19.04	kJ/mol	Joback Method
hf	-263.51	kJ/mol	Joback Method
hfus	32.74	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.913		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
tb	559.25	K	Joback Method
tc	748.13	K	Joback Method
tf	403.26	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.14	J/mol×K	559.25	Joback Method
cpg	443.28	J/mol×K	590.73	Joback Method
cpg	457.78	J/mol×K	622.21	Joback Method
cpg	471.65	J/mol×K	653.69	Joback Method
cpg	484.89	J/mol×K	685.17	Joback Method
cpg	497.51	J/mol×K	716.65	Joback Method
cpg	509.52	J/mol×K	748.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15860545&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume