valeric acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C10H14O2/c1-3-5-7-9-12-10(11)8-6-4-2/h1,5,7H,4,6,8-9H2,2H3/b7-5+
InchiKey: KMSAKRDDKNAIBK-FNORWQNLSA-N
Formula: C10H14O2
SMILES: C#C/C=C/COC(=O)CCCC
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
hf	-182.98	kJ/mol	Cheméo Relay (1.0)
hfus	27.62	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Cheméo Relay (1.0)
ie	9.19	eV	Cheméo Relay (1.0)
log10ws	-2.77		Cheméo Relay (1.0)
logp	1.909		Crippen Method
mcvol	146.300	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1241.60		NIST Webbook
tb	466.60	K	Cheméo Relay (1.0)
tc	663.95	K	Cheméo Relay (1.0)
tf	273.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.28	J/mol×K	498.77	Joback Method
cpg	328.81	J/mol×K	530.74	Joback Method
cpg	340.73	J/mol×K	562.71	Joback Method
cpg	352.07	J/mol×K	594.67	Joback Method
cpg	362.86	J/mol×K	626.64	Joback Method
cpg	373.10	J/mol×K	658.61	Joback Method
cpg	382.82	J/mol×K	690.58	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292486&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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