Fumaric acid, 2-pentyl but-3-yn-2-yl ester

Inchi: InChI=1S/C13H18O4/c1-5-7-11(4)17-13(15)9-8-12(14)16-10(3)6-2/h2,8-11H,5,7H2,1,3-4
InchiKey: DDRZURWLGFNVFB-CMDGGOBGSA-N
Formula: C13H18O4
SMILES: C#CC(C)OC(=O)C=CC(=O)OC(C)CCC
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-110.85	kJ/mol	Joback Method
hf	-402.69	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	61.88	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	1.839		Crippen Method
mcvol	196.010	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	642.82	K	Joback Method
tc	841.24	K	Joback Method
tf	392.48	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.83	J/mol×K	642.82	Joback Method
cpg	516.95	J/mol×K	675.89	Joback Method
cpg	530.30	J/mol×K	708.96	Joback Method
cpg	542.92	J/mol×K	742.03	Joback Method
cpg	554.81	J/mol×K	775.10	Joback Method
cpg	566.00	J/mol×K	808.17	Joback Method
cpg	576.50	J/mol×K	841.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405558&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume