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

Inchi: InChI=1S/C14H20O4/c1-5-11(4)18-14(16)9-8-13(15)17-10-12(6-2)7-3/h1,8-9,11-12H,6-7
InchiKey: DNKIKGCRSROOPG-CMDGGOBGSA-N
Formula: C14H20O4
SMILES: C#CC(C)OC(=O)C=CC(=O)OCC(CC)CC
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-102.43	kJ/mol	Joback Method
hf	-423.33	kJ/mol	Joback Method
hfus	33.72	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.087		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	665.70	K	Joback Method
tc	861.80	K	Joback Method
tf	403.75	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.42	J/mol×K	665.70	Joback Method
cpg	569.07	J/mol×K	698.38	Joback Method
cpg	582.94	J/mol×K	731.07	Joback Method
cpg	596.03	J/mol×K	763.75	Joback Method
cpg	608.37	J/mol×K	796.43	Joback Method
cpg	619.97	J/mol×K	829.12	Joback Method
cpg	630.86	J/mol×K	861.80	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U405631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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