Fumaric acid, 2,4,4-trimethylpentyl but-3-yn-2-yl ester

Inchi: InChI=1S/C16H24O4/c1-7-13(3)20-15(18)9-8-14(17)19-11-12(2)10-16(4,5)6/h1,8-9,12-13

InchiKey: DWGKLESWGRNXMF-CMDGGOBGSA-N

Formula: C16H24O4

SMILES: C#CC(C)OC(=O)C=CC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-82.75	kJ/mol	Joback Method
hf	-473.36	kJ/mol	Joback Method
hfus	31.49	kJ/mol	Joback Method
hvap	67.27	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.723		Crippen Method
mcvol	238.280	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	708.23	K	Joback Method
tc	909.23	K	Joback Method
tf	428.71	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.98	J/mol×K	708.23	Joback Method
cpg	679.94	J/mol×K	741.73	Joback Method
cpg	694.95	J/mol×K	775.23	Joback Method
cpg	709.05	J/mol×K	808.73	Joback Method
cpg	722.27	J/mol×K	842.23	Joback Method
cpg	734.67	J/mol×K	875.73	Joback Method
cpg	746.27	J/mol×K	909.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405600&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