Fumaric acid, 3-methylbutyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C15H22O4/c1-5-7-13(6-2)19-15(17)9-8-14(16)18-11-10-12(3)4/h8-9,12-13H,6,

InchiKey: SONHRYHTAHHGHU-CMDGGOBGSA-N

Formula: C15H22O4

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

Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-114.28	kJ/mol	Joback Method
hf	-463.57	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	68.63	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.477		Crippen Method
mcvol	224.190	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	707.46	K	Joback Method
tc	909.43	K	Joback Method
tf	474.15	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.66	J/mol×K	707.46	Joback Method
cpg	626.20	J/mol×K	741.12	Joback Method
cpg	640.87	J/mol×K	774.78	Joback Method
cpg	654.68	J/mol×K	808.44	Joback Method
cpg	667.64	J/mol×K	842.10	Joback Method
cpg	679.78	J/mol×K	875.77	Joback Method
cpg	691.09	J/mol×K	909.43	Joback Method

Sources

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=U405549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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