Fumaric acid, 2-ethylbutyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H24O4/c1-5-9-14(8-4)20-16(18)11-10-15(17)19-12-13(6-2)7-3/h10-11,13-1
InchiKey: ZUXGJJJOTWIDJG-ZHACJKMWSA-N
Formula: C16H24O4
SMILES: CC#CC(CC)OC(=O)C=CC(=O)OCC(CC)CC
Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-105.86	kJ/mol	Joback Method
hf	-484.21	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.867		Crippen Method
mcvol	238.280	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	730.34	K	Joback Method
tc	930.35	K	Joback Method
tf	485.42	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.41	J/mol×K	730.34	Joback Method
cpg	681.34	J/mol×K	763.68	Joback Method
cpg	696.36	J/mol×K	797.01	Joback Method
cpg	710.49	J/mol×K	830.35	Joback Method
cpg	723.74	J/mol×K	863.68	Joback Method
cpg	736.14	J/mol×K	897.02	Joback Method
cpg	747.69	J/mol×K	930.35	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=U405632&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