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

Inchi: InChI=1S/C18H28O4/c1-7-9-15(8-2)22-17(20)11-10-16(19)21-13-14(3)12-18(4,5)6/h10-1
InchiKey: YDESRAGTKNNVKN-ZHACJKMWSA-N
Formula: C18H28O4
SMILES: CC#CC(CC)OC(=O)C=CC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-86.18	kJ/mol	Joback Method
hf	-534.24	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	74.01	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.503		Crippen Method
mcvol	266.460	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
tb	772.87	K	Joback Method
tc	977.74	K	Joback Method
tf	510.38	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.96	J/mol×K	772.87	Joback Method
cpg	796.84	J/mol×K	807.02	Joback Method
cpg	812.68	J/mol×K	841.16	Joback Method
cpg	827.52	J/mol×K	875.31	Joback Method
cpg	841.40	J/mol×K	909.45	Joback Method
cpg	854.35	J/mol×K	943.60	Joback Method
cpg	866.43	J/mol×K	977.74	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405605&Units=SI

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