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

Inchi: InChI=1S/C18H28O4/c1-5-8-9-10-12-15(4)21-17(19)13-14-18(20)22-16(7-3)11-6-2/h13-1
InchiKey: UYFCAVVQALYUJP-BUHFOSPRSA-N
Formula: C18H28O4
SMILES: CC#CC(CC)OC(=O)C=CC(=O)OC(C)CCCCCC
Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-89.02	kJ/mol	Joback Method
hf	-525.49	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.790		Crippen Method
mcvol	266.460	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2066.00		NIST Webbook
rinpol	2066.00		NIST Webbook
tb	776.10	K	Joback Method
tc	973.70	K	Joback Method
tf	507.96	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.28	J/mol×K	776.10	Joback Method
cpg	794.85	J/mol×K	809.03	Joback Method
cpg	810.44	J/mol×K	841.97	Joback Method
cpg	825.08	J/mol×K	874.90	Joback Method
cpg	838.79	J/mol×K	907.83	Joback Method
cpg	851.58	J/mol×K	940.76	Joback Method
cpg	863.49	J/mol×K	973.70	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=U405586&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