Sebacic acid, but-3-yn-2-yl octyl ester

Inchi: InChI=1S/C22H38O4/c1-4-6-7-8-13-16-19-25-21(23)17-14-11-9-10-12-15-18-22(24)26-2
InchiKey: CVJWVMVFLQGXEN-UHFFFAOYSA-N
Formula: C22H38O4
SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-112.85	kJ/mol	Joback Method
hf	-700.39	kJ/mol	Joback Method
hfus	57.76	kJ/mol	Joback Method
hvap	82.35	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.576		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2489.00		NIST Webbook
tb	845.02	K	Joback Method
tc	1036.58	K	Joback Method
tf	513.99	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.77	J/mol×K	845.02	Joback Method
cpg	1052.81	J/mol×K	876.95	Joback Method
cpg	1069.74	J/mol×K	908.87	Joback Method
cpg	1085.59	J/mol×K	940.80	Joback Method
cpg	1100.39	J/mol×K	972.73	Joback Method
cpg	1114.17	J/mol×K	1004.66	Joback Method
cpg	1126.96	J/mol×K	1036.58	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=U355850&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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