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

Inchi: InChI=1S/C20H34O4/c1-5-18(4)24-20(22)15-11-9-7-6-8-10-14-19(21)23-16-12-13-17(2)3
InchiKey: AOCYHYCWKKKTCX-UHFFFAOYSA-N
Formula: C20H34O4
SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-132.13	kJ/mol	Joback Method
hf	-664.39	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.652		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	798.82	K	Joback Method
tc	986.75	K	Joback Method
tf	476.45	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.74	J/mol×K	798.82	Joback Method
cpg	932.17	J/mol×K	830.14	Joback Method
cpg	948.59	J/mol×K	861.46	Joback Method
cpg	964.01	J/mol×K	892.78	Joback Method
cpg	978.46	J/mol×K	924.11	Joback Method
cpg	991.96	J/mol×K	955.43	Joback Method
cpg	1004.54	J/mol×K	986.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355847&Units=SI
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

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